



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:32 AM UTC

PDB ID : 5AJ4 / pdb_00005aj4
EMDB ID : EMD-2914
Title : Structure of the 55S mammalian mitoribosome.
Authors : Greber, B.J.; Bieri, P.; Leibundgut, M.; Leitner, A.; Aebersold, R.; Boehringer, D.; Ban, N.
Deposited on : 2015-02-20
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

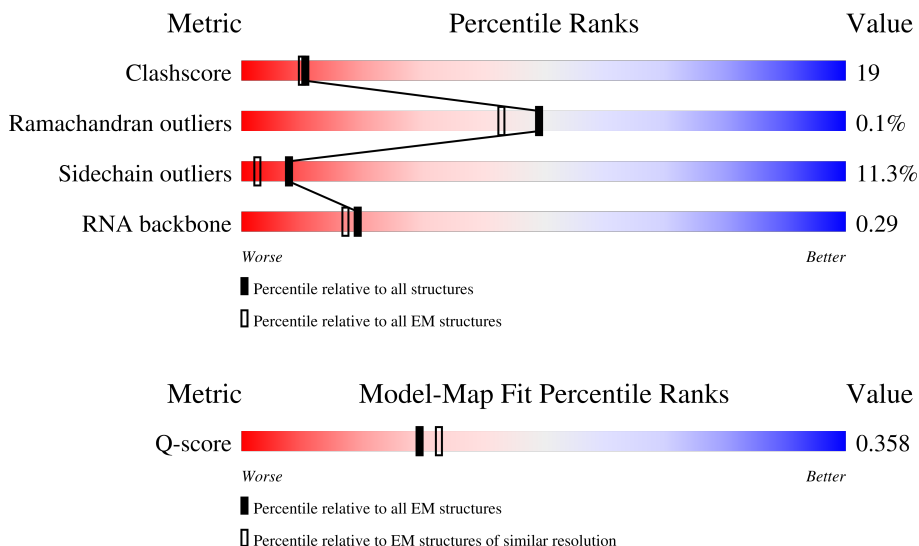
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	962	
2	AB	220	
3	AC	132	

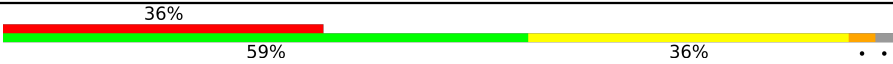
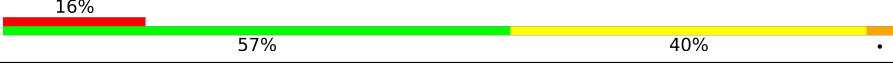
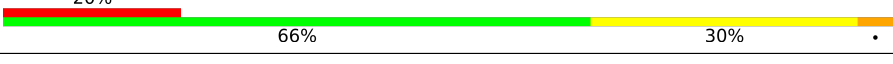
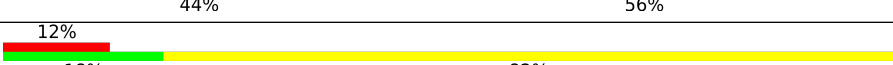
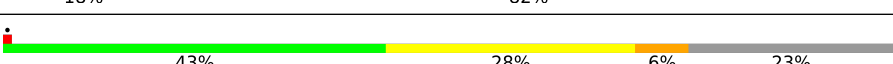
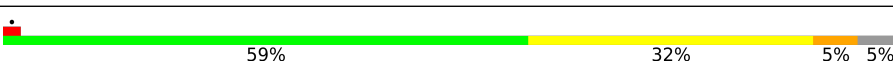
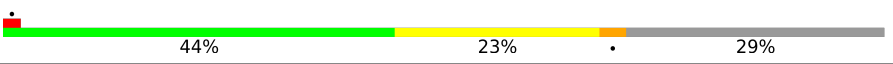
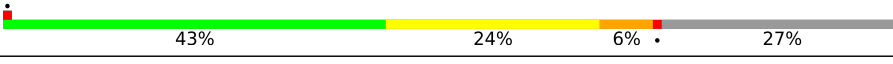
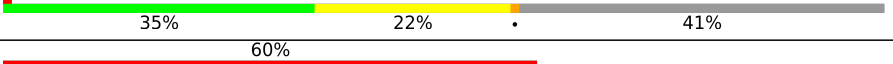
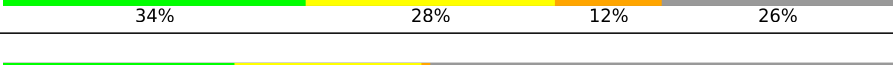
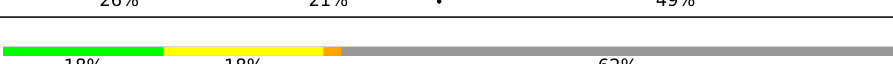
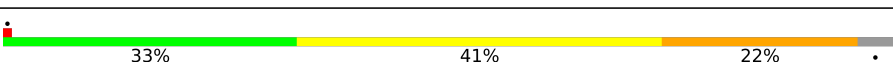
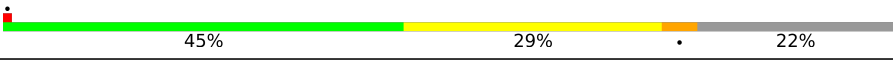
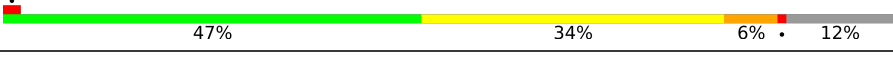
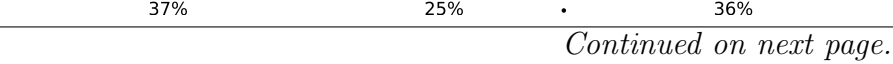
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Mol	Chain	Length	Quality of chain
4	AE	328	
5	AF	124	
6	AG	208	
7	AI	311	
8	AJ	201	
9	AK	136	
10	AL	109	
11	AN	128	
12	AO	239	
13	AP	117	
14	AQ	109	
15	AR	97	
16	AU	86	
17	AV	69	
17	AY	69	
18	AX	13	
19	Aa	356	
20	Ab	190	
21	Ac	169	
22	Ad	177	
23	Ae	336	
24	Af	188	
25	Ag	397	
26	Ah	103	
27	Ai	99	

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Mol	Chain	Length	Quality of chain
28	Aj	218	
29	Ak	275	
30	Am	116	
31	An	72	
32	Ao	530	
33	Ap	188	
34	As	16	
35	Az	17	
36	B0	148	
37	B1	256	
38	B2	252	
39	B3	161	
40	B4	126	
41	B5	188	
42	B6	65	
43	B7	95	
44	B8	188	
45	B9	100	
46	BA	1570	
47	BB	51	
48	BD	306	
49	BE	348	
50	BF	294	
51	BI	268	
52	BJ	262	

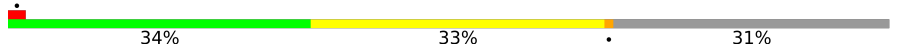
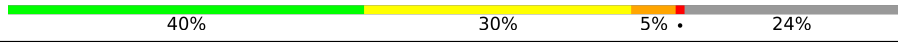
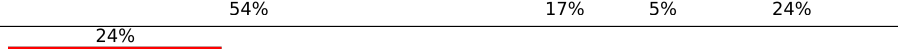
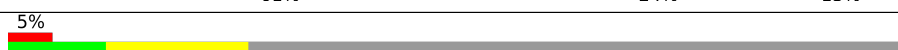
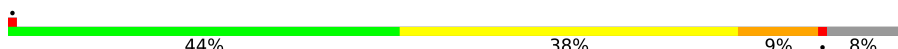
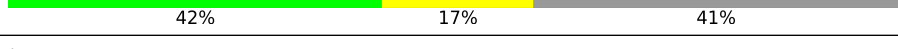
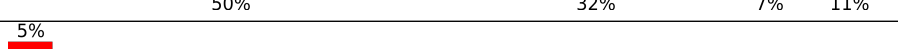
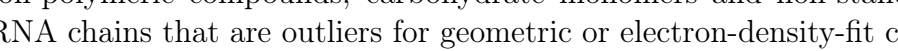
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Mol	Chain	Length	Quality of chain
53	BK	192	
54	BN	178	
55	BO	145	
56	BP	296	
57	BQ	251	
58	BR	169	
59	BS	180	
60	BT	292	
61	BU	149	
62	BV	209	
63	BW	210	
64	BX	150	
65	BY	216	
66	Ba	423	
67	Bb	380	
68	Bc	334	
69	Bd	206	
70	Be	135	
71	Bf	142	
72	Bg	159	
73	Bh	332	
74	Bi	312	
75	Bj	279	
76	Bk	212	
77	Bl	166	

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Mol	Chain	Length	Quality of chain
78	Bm	159	
79	Bn	128	
80	Bo	124	
81	Bp	112	
82	Bq	138	
83	Bt	102	
84	Bu	205	
85	Bv	222	
86	Bw	433	
87	Bx	196	
88	Bz	94	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	Y5P	AV	55	-	-	X	-
17	Y5P	AY	55	-	-	X	-
17	Y5P	AY	58	-	-	X	-

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 167915 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called MITORIBOSOMAL 12S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	960	Total	C	N	O	P	0	0
			20411	9162	3708	6581	960		

- Molecule 2 is a protein called MITORIBOSOMAL PROTEIN US2M, MRPS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	220	Total	C	N	O	S	0	0
			1762	1126	326	304	6		

- Molecule 3 is a protein called MITORIBOSOMAL PROTEIN US3M, MRPS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	132	Total	C	N	O	S	0	0
			1075	695	195	181	4		

- Molecule 4 is a protein called MITORIBOSOMAL PROTEIN US5M, MRPS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AE	328	Total	C	N	O	S	0	0
			2621	1641	498	471	11		

- Molecule 5 is a protein called MITORIBOSOMAL PROTEIN BS6M, MRPS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AF	123	Total	C	N	O	S	0	0
			990	626	180	178	6		

- Molecule 6 is a protein called MITORIBOSOMAL PROTEIN US7M, MRPS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AG	208	Total	C	N	O	S	0	0
			1721	1097	314	299	11		

- Molecule 7 is a protein called MITORIBOSOMAL PROTEIN US9M, MRPS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AI	311	Total	C	N	O	S	0	0
			2498	1586	450	449	13		

- Molecule 8 is a protein called MITORIBOSOMAL PROTEIN US10M, MRPS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AJ	129	Total	C	N	O	S	0	0
			1067	690	182	192	3		

- Molecule 9 is a protein called MITORIBOSOMAL PROTEIN US11M, MRPS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AK	136	Total	C	N	O	S	0	0
			1001	628	192	178	3		

- Molecule 10 is a protein called MITORIBOSOMAL PROTEIN US12M, MRPS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AL	109	Total	C	N	O	S	0	0
			840	524	172	138	6		

- Molecule 11 is a protein called MITORIBOSOMAL PROTEIN US14M, MRPS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AN	101	Total	C	N	O	S	0	0
			858	534	174	144	6		

- Molecule 12 is a protein called MITORIBOSOMAL PROTEIN US15M, MRPS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AO	175	Total	C	N	O	S	0	0
			1448	919	272	248	9		

- Molecule 13 is a protein called MITORIBOSOMAL PROTEIN BS16M, MRPS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AP	117	Total	C	N	O	S	0	0
			932	588	184	155	5		

- Molecule 14 is a protein called MITORIBOSOMAL PROTEIN US17M, MRPS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AQ	109	Total	C	N	O	S	0	0
			853	555	150	145	3		

- Molecule 15 is a protein called MITORIBOSOMAL PROTEIN BS18M, MRPS18C.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AR	97	Total	C	N	O	S	0	0
			784	507	132	138	7		

- Molecule 16 is a protein called MITORIBOSOMAL PROTEIN BS21M, MRPS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AU	86	Total	C	N	O	S	0	0
			734	453	148	125	8		

- Molecule 17 is a RNA chain called P-SITE AND A-SITE TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AV	69	Total	C	N	O	P	0	0
			1251	625	146	412	68		
17	AY	69	Total	C	N	O	P	0	0
			1251	625	146	412	68		

- Molecule 18 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AX	13	Total	C	N	O	P	0	0
			231	117	26	76	12		

- Molecule 19 is a protein called MITORIBOSOMAL PROTEIN MS22, MRPS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Aa	292	Total	C	N	O	S	0	0
			2296	1476	394	417	9		

- Molecule 20 is a protein called MITORIBOSOMAL PROTEIN MS23, MRPS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ab	135	Total	C	N	O	S	0	0
			1101	709	199	192	1		

- Molecule 21 is a protein called MITORIBOSOMAL PROTEIN MS25, MRPS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ac	169	Total	C	N	O	S	0	0
			1367	876	236	245	10		

- Molecule 22 is a protein called MITORIBOSOMAL PROTEIN MS26, MRPS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Ad	177	Total	C	N	O	S	0	0
			1467	904	288	273	2		

- Molecule 23 is a protein called MITORIBOSOMAL PROTEIN MS27, MRPS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ae	336	Total	C	N	O	S	0	0
			2016	1344	336	336			

- Molecule 24 is a protein called MITORIBOSOMAL PROTEIN MS28, MRPS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Af	99	Total	C	N	O	S	0	0
			778	494	134	146	4		

- Molecule 25 is a protein called MITORIBOSOMAL PROTEIN MS29, MRPS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ag	346	Total	C	N	O	S	0	0
			2774	1786	489	489	10		

- Molecule 26 is a protein called MITORIBOSOMAL PROTEIN MS31, MRPS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ah	103	Total	C	N	O	S	0	0
			876	569	145	159	3		

- Molecule 27 is a protein called MITORIBOSOMAL PROTEIN MS33, MRPS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ai	99	Total	C	N	O	S	0	0
			824	522	156	143	3		

- Molecule 28 is a protein called MITORIBOSOMAL PROTEIN MS34, MRPS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Aj	213	Total	C	N	O	S	0	0
			1777	1123	339	308	7		

- Molecule 29 is a protein called MITORIBOSOMAL PROTEIN MS35, MRPS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ak	275	Total	C	N	O	S	0	0
			2222	1414	380	419	9		

- Molecule 30 is a protein called MITORIBOSOMAL PROTEIN MS37, MRPS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Am	116	Total	C	N	O	S	0	0
			930	577	185	160	8		

- Molecule 31 is a protein called MITORIBOSOMAL PROTEIN MS38, MRPS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	An	72	Total	C	N	O	S	0	0
			639	407	139	92	1		

- Molecule 32 is a protein called MITORIBOSOMAL PROTEIN MS39, MRPS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ao	476	Total	C	N	O	S	0	0
			3028	2007	500	519	2		

- Molecule 33 is a protein called 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ap	188	Total	C	N	O	S	0	0
			1551	983	290	270	8		

- Molecule 34 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	As	16	Total	C	N	O	0	0
			96	64	16	16		

- Molecule 35 is a protein called UNASSIGNED HELICES.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Az	17	Total	C	N	O	0	0
			102	68	17	17		

- Molecule 36 is a protein called MITORIBOSOMAL PROTEIN BL27M, MRPL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B0	114	Total	C	N	O	S	0	0
			878	564	160	151	3		

- Molecule 37 is a protein called MITORIBOSOMAL PROTEIN BL28M, MRPL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B1	244	Total	C	N	O	S	0	0
			2036	1315	363	353	5		

- Molecule 38 is a protein called MITORIBOSOMAL PROTEIN UL29M, MRPL47.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B2	178	Total	C	N	O	S	0	0
			1544	990	289	259	6		

- Molecule 39 is a protein called MITORIBOSOMAL PROTEIN UL30M, MRPL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B3	118	Total	C	N	O	S	0	0
			968	622	178	165	3		

- Molecule 40 is a protein called MITORIBOSOMAL PROTEIN BL31M, MRPL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B4	45	Total	C	N	O	S	0	0
			381	239	77	62	3		

- Molecule 41 is a protein called MITORIBOSOMAL PROTEIN BL32M, MRPL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B5	110	Total	C	N	O	S	0	0
			902	553	181	162	6		

- Molecule 42 is a protein called MITORIBOSOMAL PROTEIN BL33M, MRPL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B6	48	Total	C	N	O	S	0	0
			391	253	70	66	2		

- Molecule 43 is a protein called MITORIBOSOMAL PROTEIN BL34M, MRPL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	B7	46	Total	C	N	O	S	0	0
			387	239	89	58	1		

- Molecule 44 is a protein called MITORIBOSOMAL PROTEIN BL35M, MRPL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	B8	95	Total	C	N	O	S	0	0
			833	539	163	129	2		

- Molecule 45 is a protein called MITORIBOSOMAL PROTEIN BL36M, MRPL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	B9	38	Total	C	N	O	S	0	0
			335	214	70	47	4		

- Molecule 46 is a RNA chain called MITORIBOSOMAL 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BA	1515	Total	C	N	O	P	0	0
			32233	14473	5860	10385	1515		

- Molecule 47 is a RNA chain called MITORIBOSOMAL CP TRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BB	51	Total	C	N	O	P	0	0
			1008	489	162	306	51		

- Molecule 48 is a protein called MITORIBOSOMAL PROTEIN UL2M, MRPL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BD	240	Total	C	N	O	S	0	0
			1860	1160	371	319	10		

- Molecule 49 is a protein called MITORIBOSOMAL PROTEIN UL3M, MRPL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BE	307	Total	C	N	O	S	0	0
			2420	1554	426	430	10		

- Molecule 50 is a protein called MITORIBOSOMAL PROTEIN UL4M, MRPL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BF	250	Total	C	N	O	S	0	0
			2011	1294	367	344	6		

- Molecule 51 is a protein called MITORIBOSOMAL PROTEIN BL9M, MRPL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BI	98	Total	C	N	O	S	0	0
			805	509	155	141			

- Molecule 52 is a protein called MITORIBOSOMAL PROTEIN UL10M, MRPL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BJ	168	Total	C	N	O	S	0	0
			1361	879	248	226	8		

- Molecule 53 is a protein called MITORIBOSOMAL PROTEIN UL11M, MRPL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BK	142	Total	C	N	O	S	0	0
			1081	690	197	192	2		

- Molecule 54 is a protein called MITORIBOSOMAL PROTEIN UL13M, MRPL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BN	177	Total	C	N	O	S	0	0
			1444	926	258	253	7		

- Molecule 55 is a protein called MITORIBOSOMAL PROTEIN UL14M, MRPL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BO	115	Total	C	N	O	S	0	0
			896	562	176	154	4		

- Molecule 56 is a protein called MITORIBOSOMAL PROTEIN UL15M, MRPL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BP	288	Total	C	N	O	S	0	0
			2312	1473	430	403	6		

- Molecule 57 is a protein called MITORIBOSOMAL PROTEIN UL16M, MRPL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BQ	221	Total	C	N	O	S	0	0
			1792	1147	330	305	10		

- Molecule 58 is a protein called MITORIBOSOMAL PROTEIN BL17M, MRPL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BR	153	Total	C	N	O	S	0	0
			1240	777	236	222	5		

- Molecule 59 is a protein called MITORIBOSOMAL PROTEIN UL18M, MRPL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BS	143	Total	C	N	O	S	0	0
			1168	733	227	204	4		

- Molecule 60 is a protein called MITORIBOSOMAL PROTEIN BL19M, MRPL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BT	239	Total	C	N	O	S	0	0
			1950	1249	339	353	9		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	54	UNK	PHE	conflict	UNP I3LNJ0
BT	55	UNK	GLN	conflict	UNP I3LNJ0
BT	56	UNK	PRO	conflict	UNP I3LNJ0
BT	57	UNK	PRO	conflict	UNP I3LNJ0
BT	58	UNK	PRO	conflict	UNP I3LNJ0
BT	59	UNK	LYS	conflict	UNP I3LNJ0
BT	60	UNK	PRO	conflict	UNP I3LNJ0
BT	61	UNK	VAL	conflict	UNP I3LNJ0
BT	62	UNK	ILE	conflict	UNP I3LNJ0
BT	63	UNK	VAL	conflict	UNP I3LNJ0
BT	64	UNK	ASP	conflict	UNP I3LNJ0
BT	65	UNK	LYS	conflict	UNP I3LNJ0

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Chain	Residue	Modelled	Actual	Comment	Reference
BT	66	UNK	ARG	conflict	UNP I3LNJ0
BT	67	UNK	ARG	conflict	UNP I3LNJ0
BT	68	UNK	PRO	conflict	UNP I3LNJ0

- Molecule 61 is a protein called MITORIBOSOMAL PROTEIN BL20M, MRPL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BU	140	Total	C	N	O	S	0	0
			1159	732	239	185	3		

- Molecule 62 is a protein called MITORIBOSOMAL PROTEIN BL21M, MRPL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BV	155	Total	C	N	O	S	0	0
			1231	789	219	219	4		

- Molecule 63 is a protein called MITORIBOSOMAL PROTEIN UL22M, MRPL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BW	166	Total	C	N	O	S	0	0
			1374	876	258	234	6		

- Molecule 64 is a protein called MITORIBOSOMAL PROTEIN UL23M, MRPL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BX	134	Total	C	N	O	S	0	0
			1120	715	217	186	2		

- Molecule 65 is a protein called MITORIBOSOMAL PROTEIN UL24M, MRPL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	BY	204	Total	C	N	O	S	0	0
			1663	1047	305	306	5		

- Molecule 66 is a protein called MITORIBOSOMAL PROTEIN ML37, MRPL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ba	393	Total	C	N	O	S	0	0
			3173	2040	556	565	12		

- Molecule 67 is a protein called MITORIBOSOMAL PROTEIN ML38, MRPL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bb	354	Total	C	N	O	S	0	0
			2952	1876	542	525	9		

- Molecule 68 is a protein called MITORIBOSOMAL PROTEIN ML39, MRPL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bc	295	Total	C	N	O	S	0	0
			2408	1541	410	441	16		

- Molecule 69 is a protein called MITORIBOSOMAL PROTEIN ML40, MRPL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bd	99	Total	C	N	O	S	0	0
			832	528	148	155	1		

- Molecule 70 is a protein called MITORIBOSOMAL PROTEIN ML41, MRPL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Be	121	Total	C	N	O	S	0	0
			968	626	167	172	3		

- Molecule 71 is a protein called MITORIBOSOMAL PROTEIN ML42, MRPL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bf	108	Total	C	N	O	S	0	0
			852	544	154	150	4		

- Molecule 72 is a protein called MITORIBOSOMAL PROTEIN ML43, MRPL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bg	148	Total	C	N	O	S	0	0
			1167	727	225	212	3		

- Molecule 73 is a protein called MITORIBOSOMAL PROTEIN ML44, MRPL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bh	289	Total	C	N	O	S	0	0
			2319	1486	399	426	8		

- Molecule 74 is a protein called MITORIBOSOMAL PROTEIN ML45, MRPL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bi	242	Total	C	N	O	S	0	0
			1979	1266	352	351	10		

- Molecule 75 is a protein called MITORIBOSOMAL PROTEIN ML46, MRPL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bj	217	Total	C	N	O	S	0	0
			1775	1137	311	321	6		

- Molecule 76 is a protein called MITORIBOSOMAL PROTEIN ML48, MRPL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bk	136	Total	C	N	O	S	0	0
			1087	692	185	205	5		

- Molecule 77 is a protein called MITORIBOSOMAL PROTEIN ML49, MRPL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bl	133	Total	C	N	O	S	0	0
			1097	709	192	194	2		

- Molecule 78 is a protein called MITORIBOSOMAL PROTEIN ML50, MRPL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bm	109	Total	C	N	O	S	0	0
			893	568	160	162	3		

- Molecule 79 is a protein called MITORIBOSOMAL PROTEIN ML51, MRPL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bn	97	Total	C	N	O	S	0	0
			837	539	166	128	4		

- Molecule 80 is a protein called MITORIBOSOMAL PROTEIN ML52, MRPL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bo	94	Total	C	N	O	S	0	0
			747	466	143	136	2		

- Molecule 81 is a protein called MITORIBOSOMAL PROTEIN ML53, MRPL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bp	97	Total	C	N	O	S	0	0
			742	459	143	134	6		

- Molecule 82 is a protein called MITORIBOSOMAL PROTEIN ML54, MRPL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
82	Bq	37	Total	C	N	O	0	0
			336	214	69	53		

- Molecule 83 is a protein called MITORIBOSOMAL PROTEIN ML63, MRPL57.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Bt	94	Total	C	N	O	S	0	0
			780	485	168	126	1		

- Molecule 84 is a protein called MITORIBOSOMAL PROTEIN ML62, MRPL58.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bu	151	Total	C	N	O	S	0	0
			1208	748	233	222	5		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bu	164	UNK	ALA	conflict	UNP W5IDC0
Bu	165	UNK	LYS	conflict	UNP W5IDC0
Bu	166	UNK	GLU	conflict	UNP W5IDC0
Bu	167	UNK	PRO	conflict	UNP W5IDC0
Bu	168	UNK	SER	conflict	UNP W5IDC0
Bu	169	UNK	ARG	conflict	UNP W5IDC0
Bu	170	UNK	GLU	conflict	UNP W5IDC0
Bu	171	UNK	ASP	conflict	UNP W5IDC0
Bu	172	UNK	ALA	conflict	UNP W5IDC0
Bu	173	UNK	GLU	conflict	UNP W5IDC0

- Molecule 85 is a protein called MITORIBOSOMAL PROTEIN ML64, MRPL59.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Bv	131	Total	C	N	O	S	0	0
			1068	662	206	195	5		

- Molecule 86 is a protein called MITORIBOSOMAL PROTEIN ML65, MRPS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Bw	387	Total	C	N	O	S	0	0
			3126	2011	548	555	12		

- Molecule 87 is a protein called MITORIBOSOMAL PROTEIN ML66, MRPS18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	Bx	162	Total	C	N	O	S	0	0
			1325	845	249	224	7		

- Molecule 88 is a protein called UNASSIGNED SECONDARY STRUCTURE ELEMENTS.

Mol	Chain	Residues	Atoms				AltConf	Trace
88	Bz	94	Total	C	N	O	0	0
			564	376	94	94		

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	AA	146	Total	Mg	0
			146	146	
89	Ag	1	Total	Mg	0
			1	1	
89	B0	1	Total	Mg	0
			1	1	
89	B2	1	Total	Mg	0
			1	1	
89	BA	195	Total	Mg	0
			195	195	
89	BD	2	Total	Mg	0
			2	2	
89	BE	1	Total	Mg	0
			1	1	
89	BP	1	Total	Mg	0
			1	1	
89	BR	2	Total	Mg	0
			2	2	
89	BX	1	Total	Mg	0
			1	1	

- Molecule 90 is ZINC ION (CCD ID: ZN) (formula: Zn).

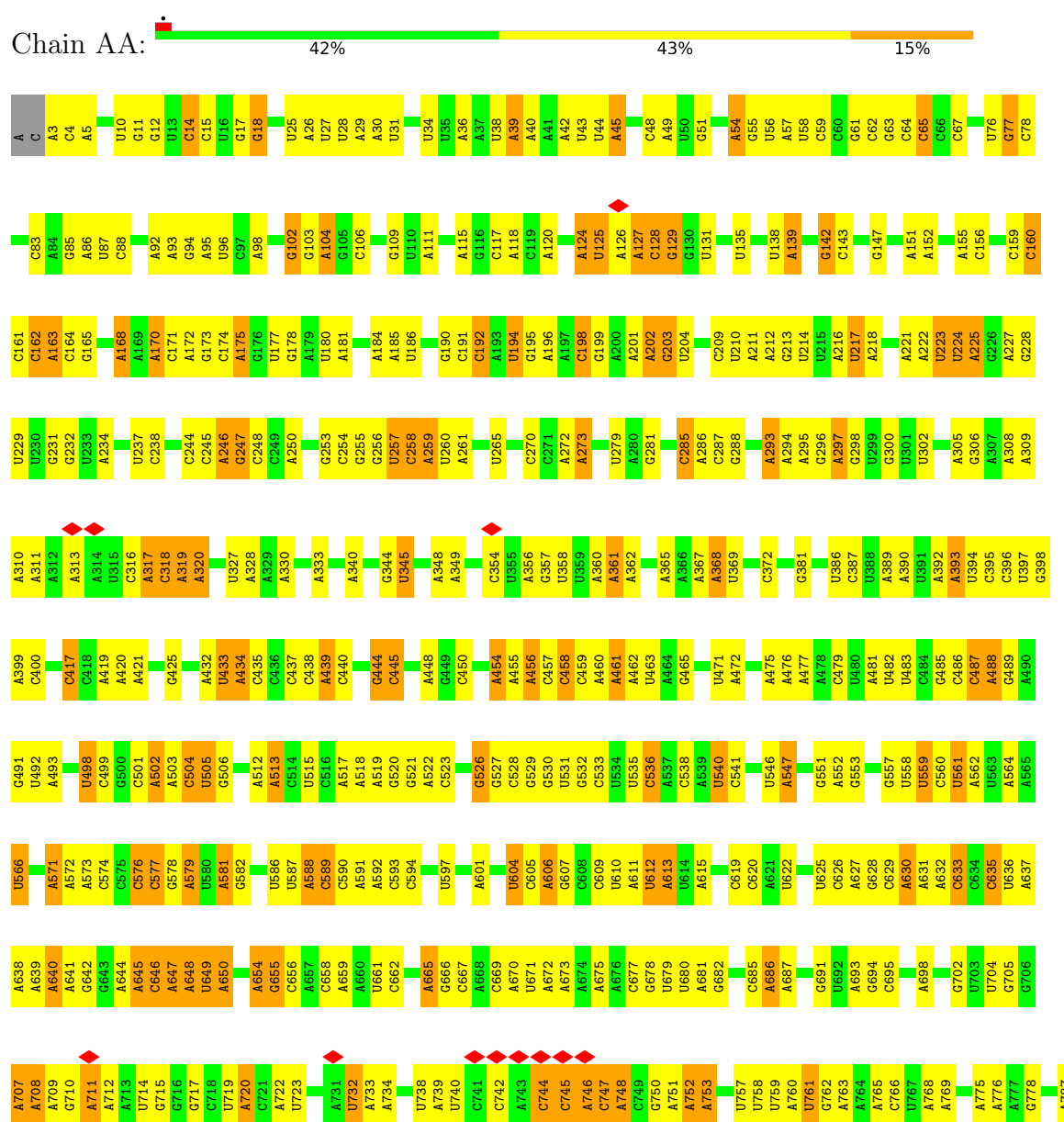
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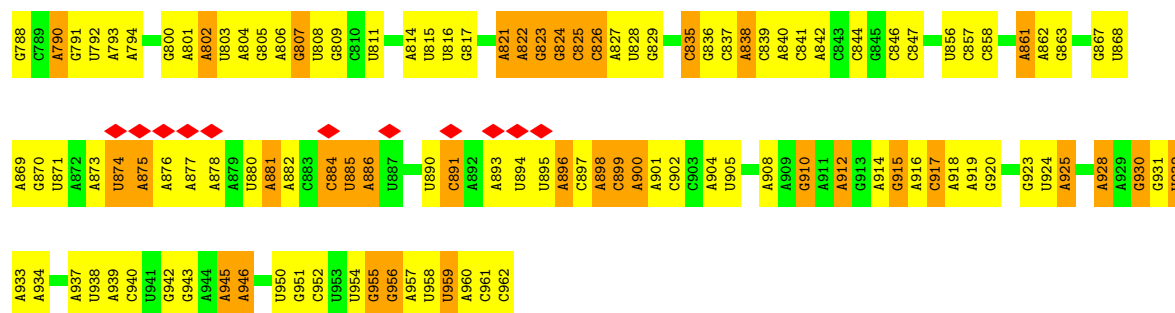
Mol	Chain	Residues	Atoms		AltConf
92	B7	2	Total 2	O 2	0
92	B8	1	Total 1	O 1	0
92	BA	196	Total 196	O 196	0
92	BD	3	Total 3	O 3	0
92	BF	4	Total 4	O 4	0
92	BI	1	Total 1	O 1	0
92	BO	2	Total 2	O 2	0
92	BP	3	Total 3	O 3	0
92	BR	2	Total 2	O 2	0
92	BU	1	Total 1	O 1	0
92	BW	4	Total 4	O 4	0

3 Residue-property plots

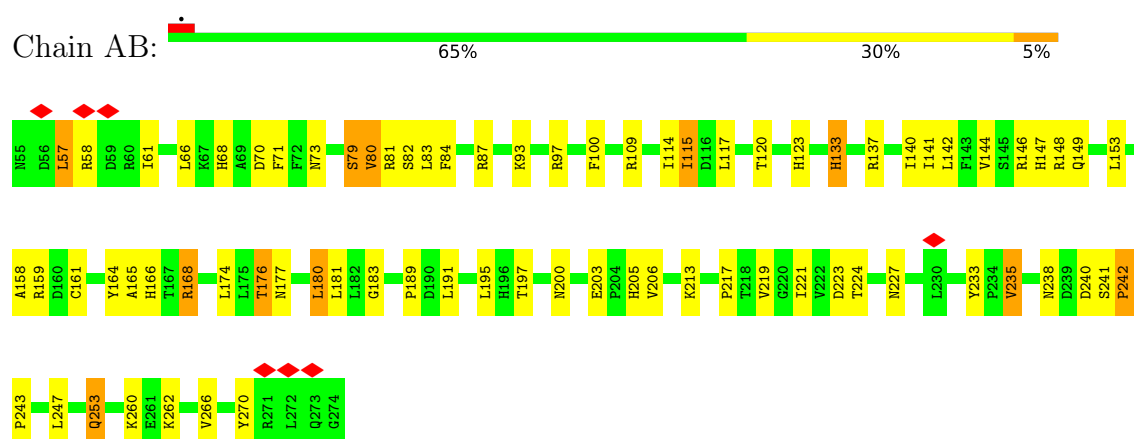
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MITORIBOSOMAL 12S Ribosomal RNA

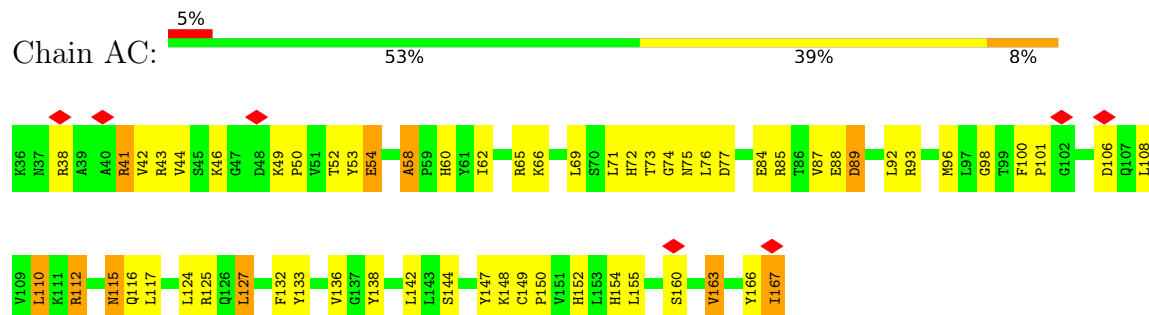




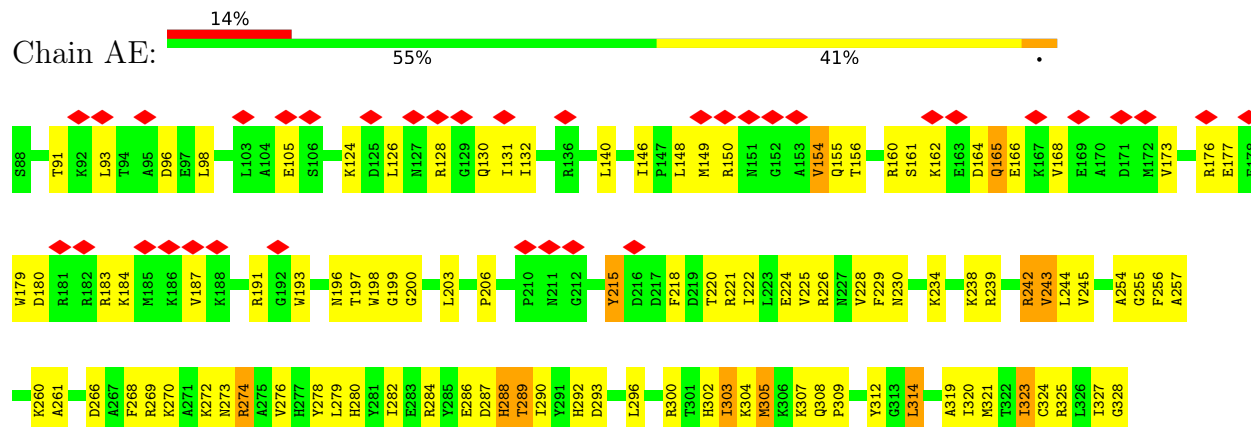
• Molecule 2: MITORIBOSOMAL PROTEIN US2M, MRPS2

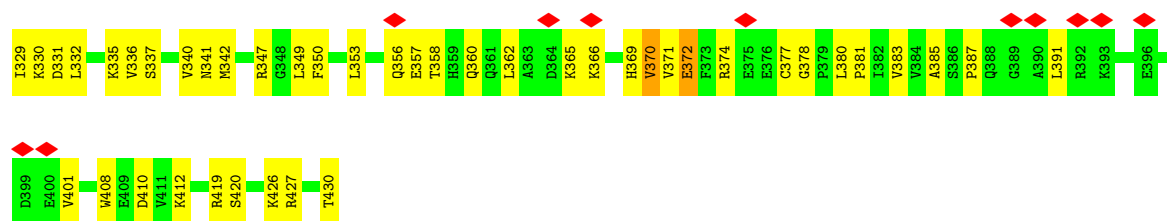


• Molecule 3: MITORIBOSOMAL PROTEIN US3M, MRPS24

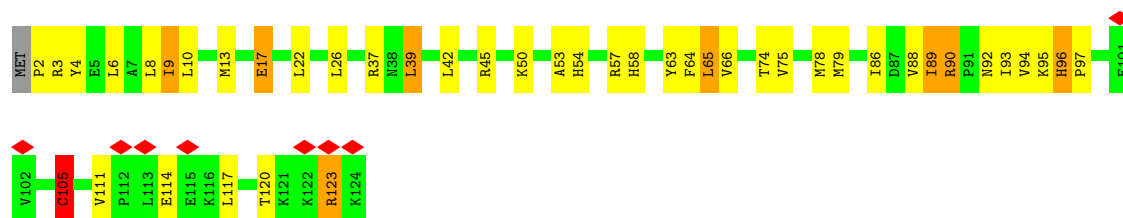


• Molecule 4: MITORIBOSOMAL PROTEIN US5M, MRPS5

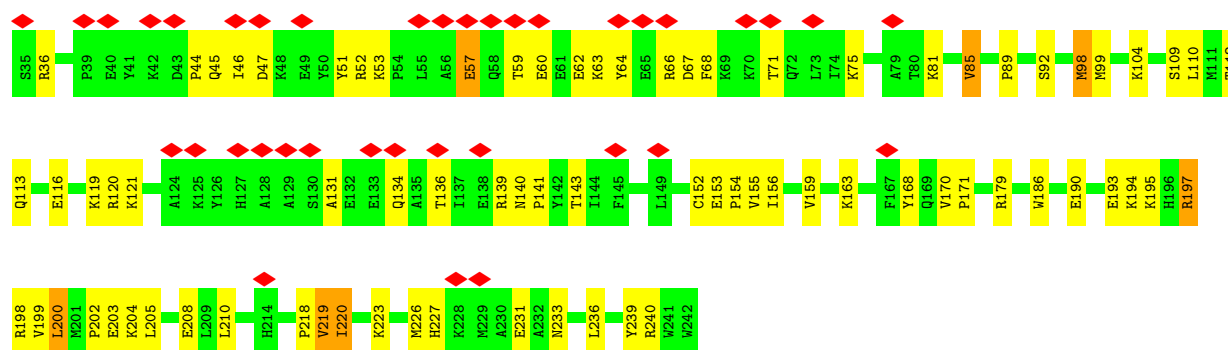




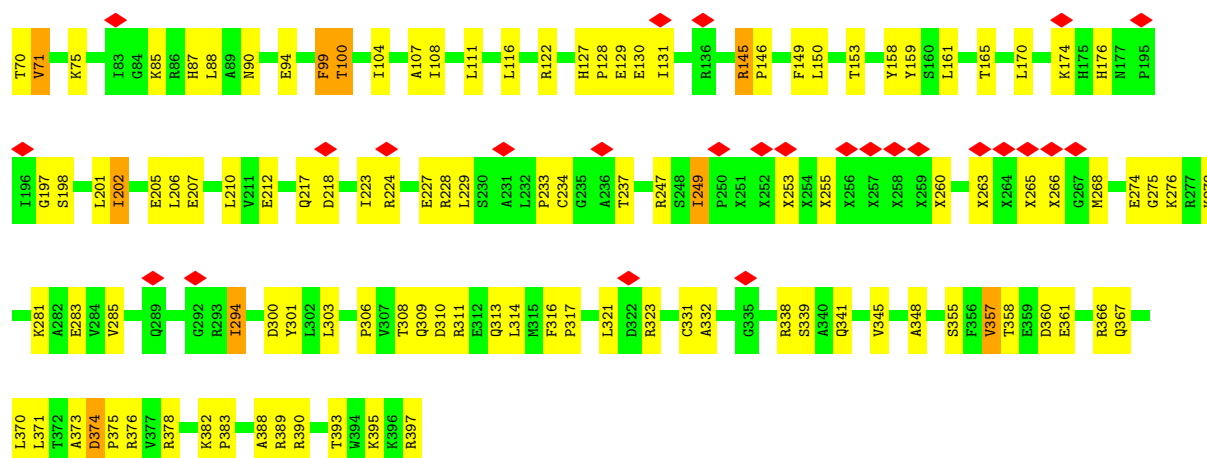
• Molecule 5: MITORIBOSOMAL PROTEIN BS6M, MRPS6



• Molecule 6: MITORIBOSOMAL PROTEIN US7M, MRPS7



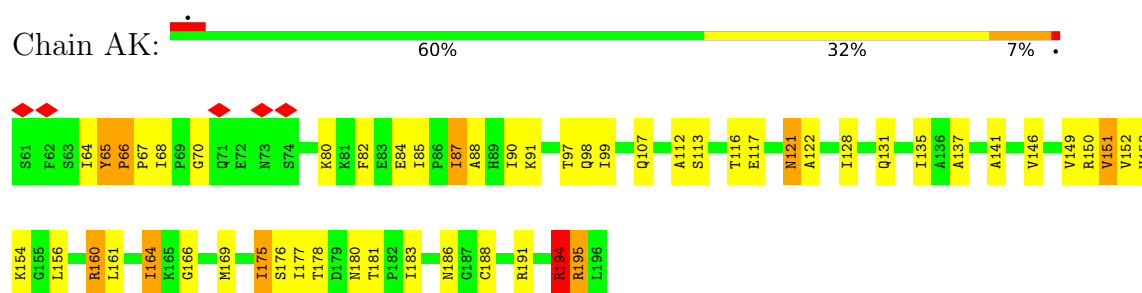
• Molecule 7: MITORIBOSOMAL PROTEIN US9M, MRPS9



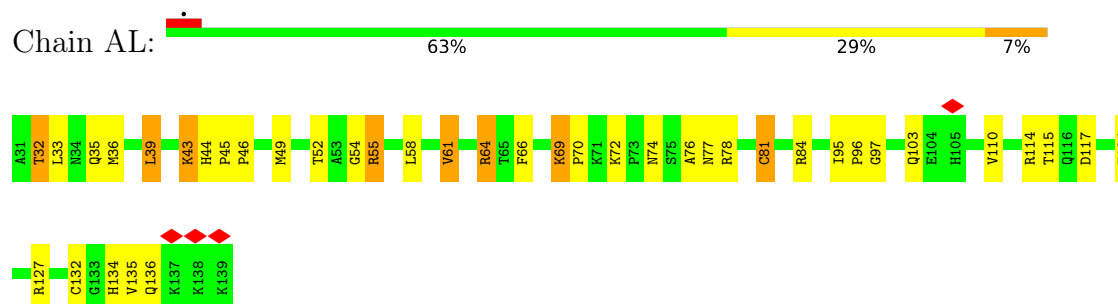
• Molecule 8: MITORIBOSOMAL PROTEIN US10M, MRPS10



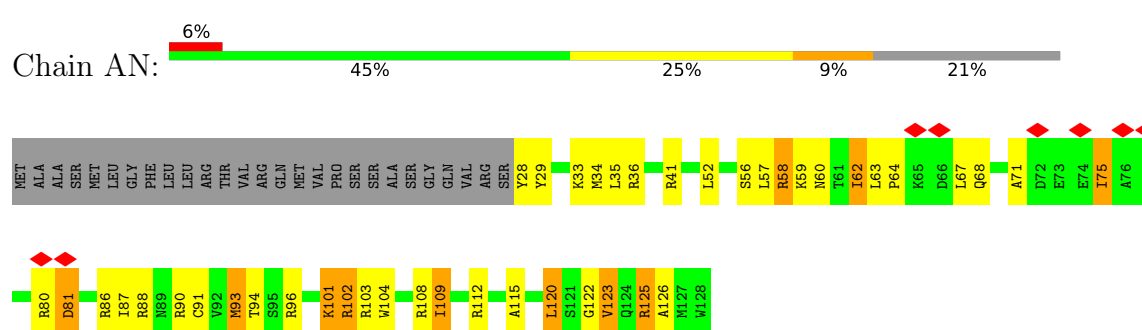
• Molecule 9: MITORIBOSOMAL PROTEIN US11M, MRPS11



• Molecule 10: MITORIBOSOMAL PROTEIN US12M, MRPS12



• Molecule 11: MITORIBOSOMAL PROTEIN US14M, MRPS14

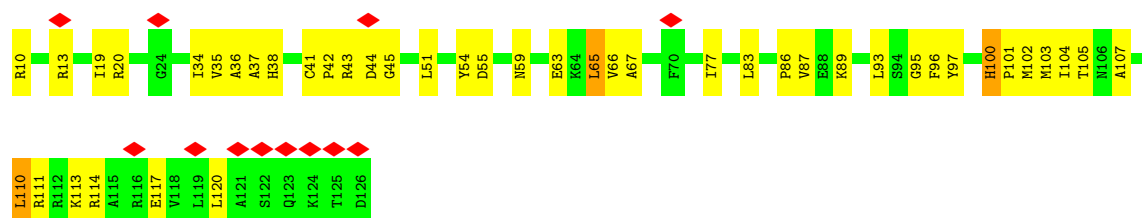


• Molecule 12: MITORIBOSOMAL PROTEIN US15M, MRPS15

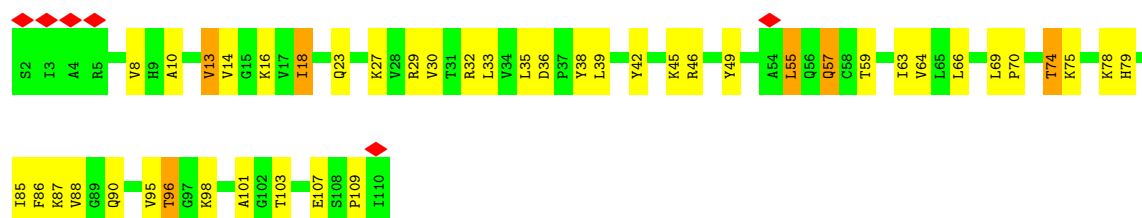




• Molecule 13: MITORIBOSOMAL PROTEIN BS16M, MRPS16



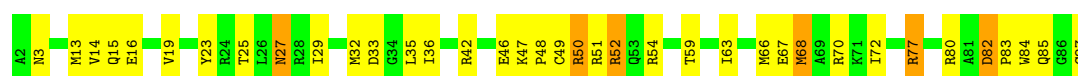
• Molecule 14: MITORIBOSOMAL PROTEIN US17M, MRPS17



• Molecule 15: MITORIBOSOMAL PROTEIN BS18M, MRPS18C

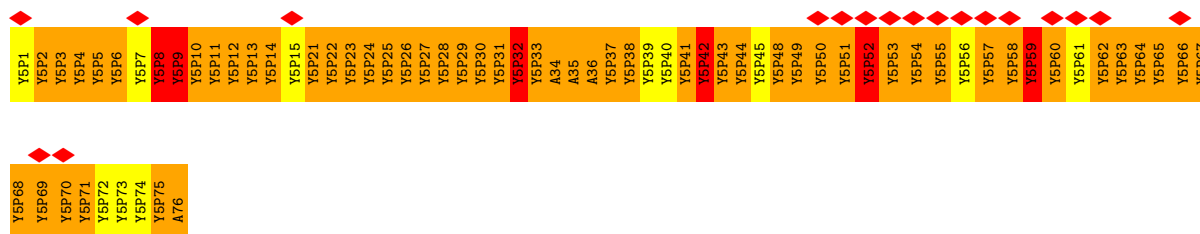


• Molecule 16: MITORIBOSOMAL PROTEIN BS21M, MRPS21



• Molecule 17: P-SITE AND A-SITE TRNA





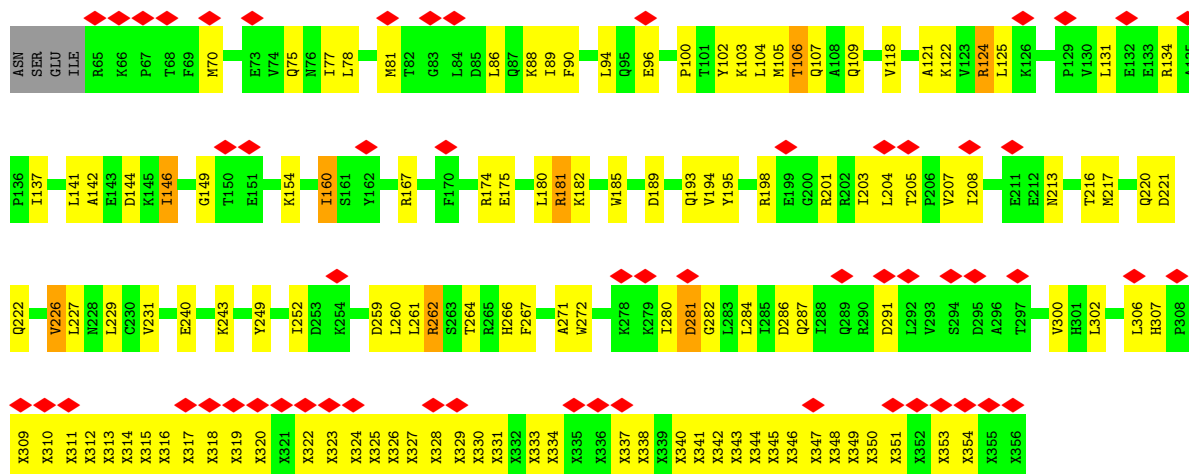
• Molecule 17: P-SITE AND A-SITE TRNA



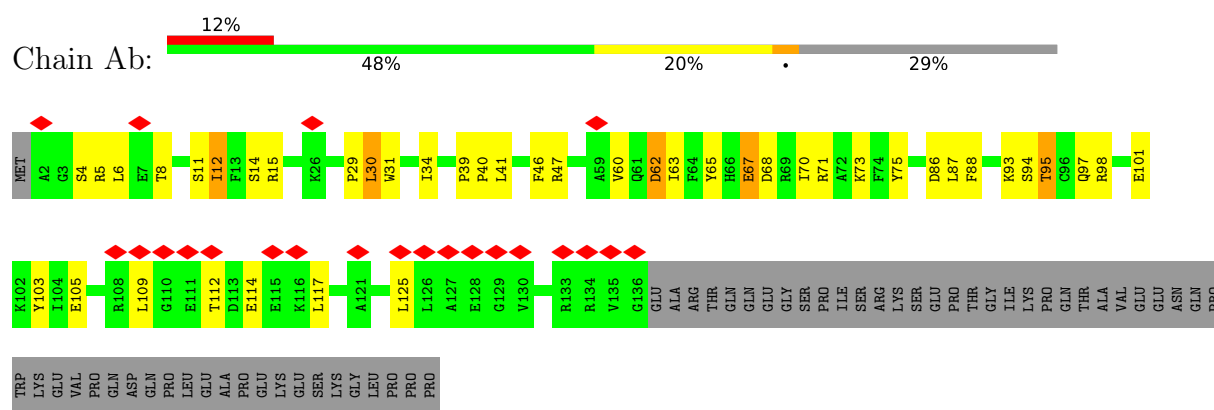
• Molecule 18: MRNA



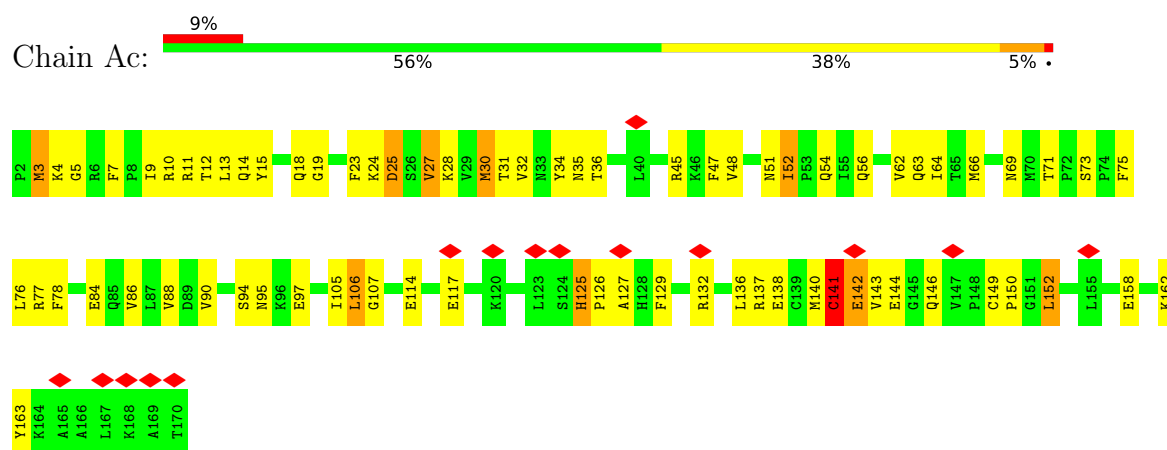
• Molecule 19: MITORIBOSOMAL PROTEIN MS22, MRPS22



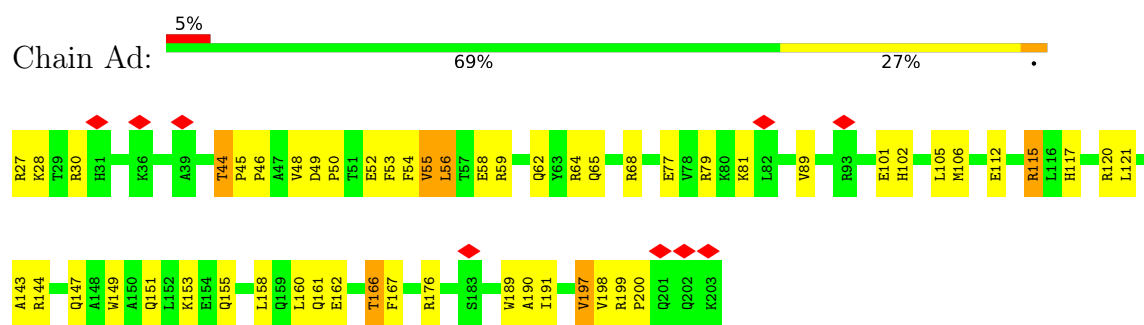
• Molecule 20: MITORIBOSOMAL PROTEIN MS23, MRPS23



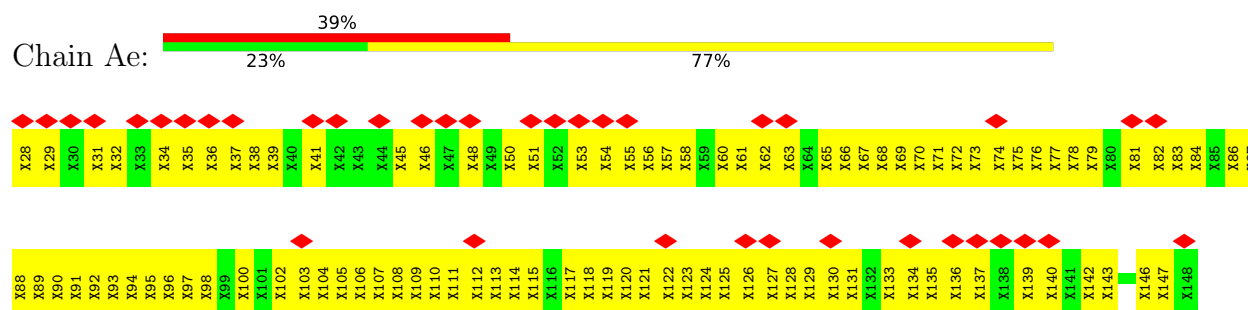
• Molecule 21: MITORIBOSOMAL PROTEIN MS25, MRPS25

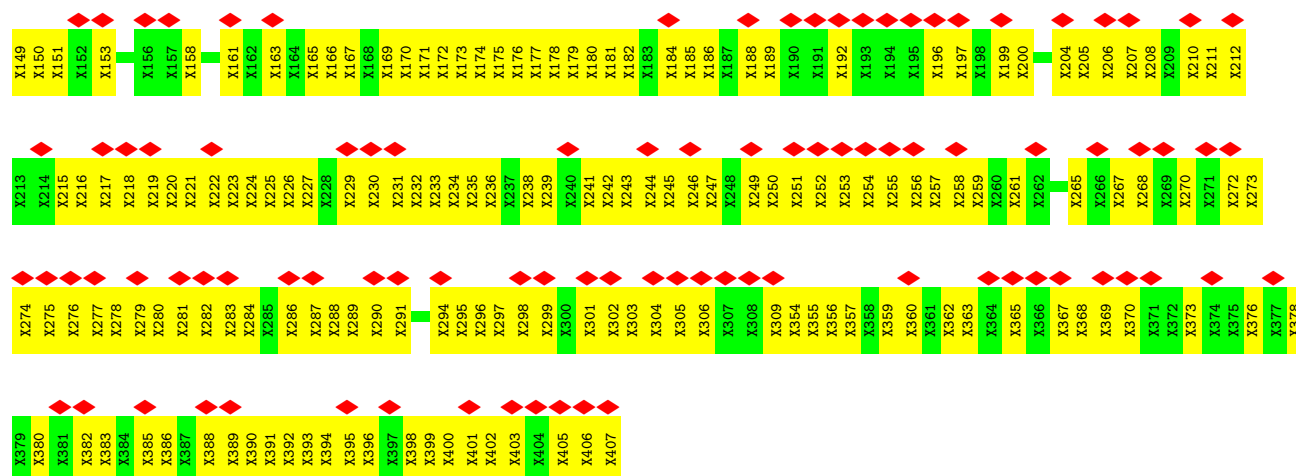


• Molecule 22: MITORIBOSOMAL PROTEIN MS26, MRPS26

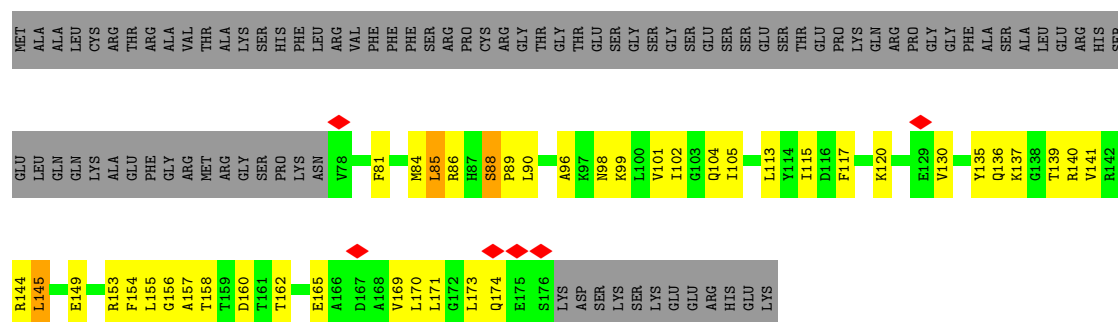
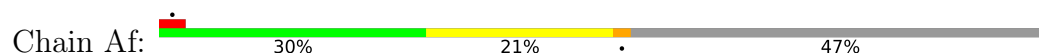


• Molecule 23: MITORIBOSOMAL PROTEIN MS27, MRPS27

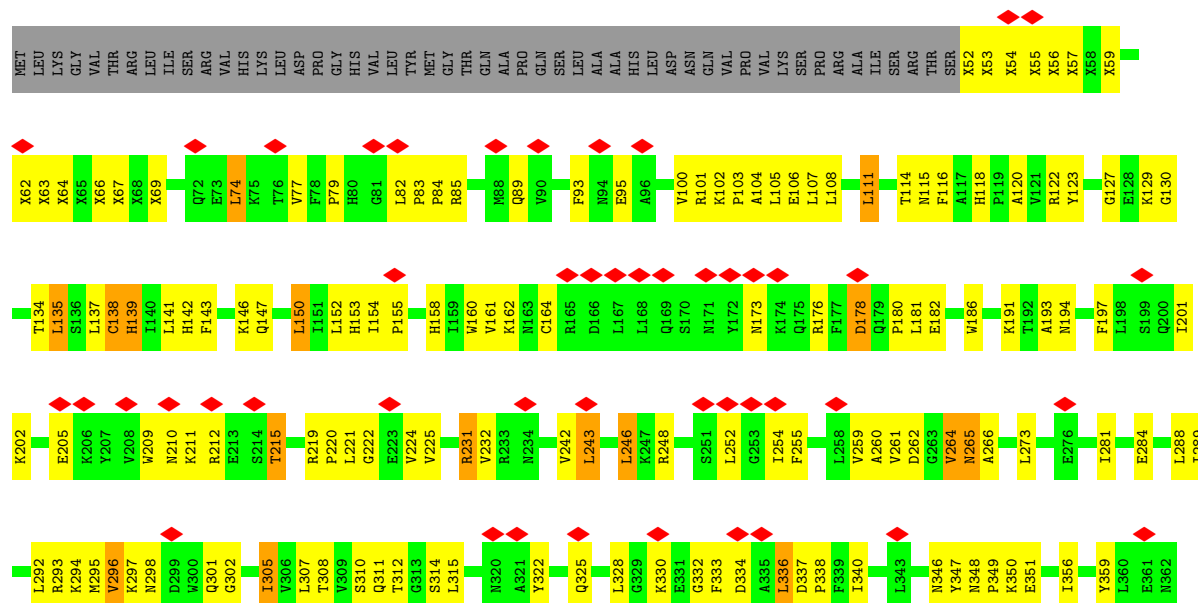


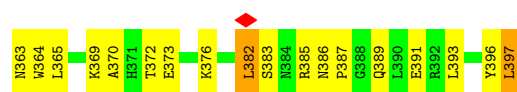


• Molecule 24: MITORIBOSOMAL PROTEIN MS28, MRPS28

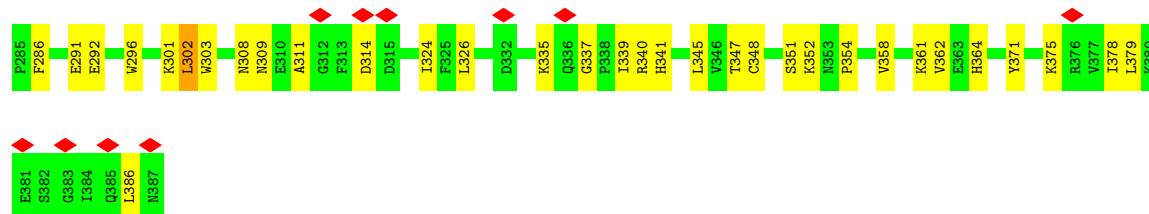


• Molecule 25: MITORIBOSOMAL PROTEIN MS29, MRPS29

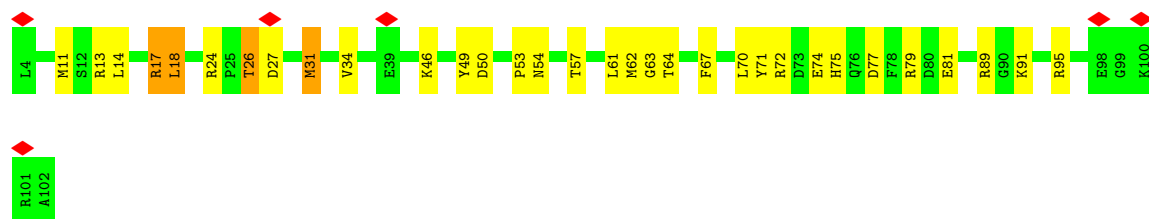




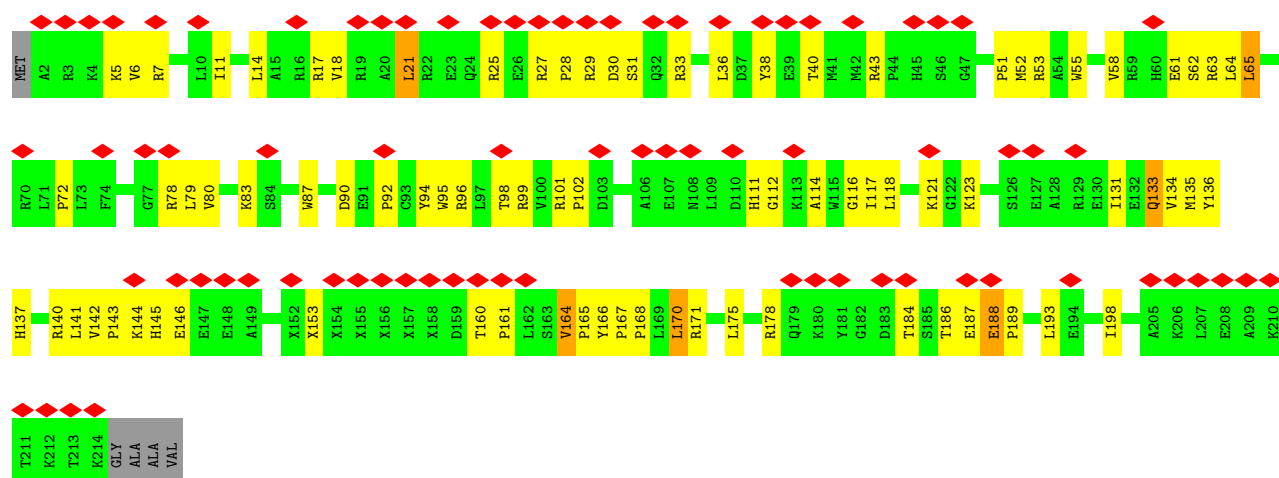
- Molecule 26: MITORIBOSOMAL PROTEIN MS31, MRPS31



- Molecule 27: MITORIBOSOMAL PROTEIN MS33, MRPS33

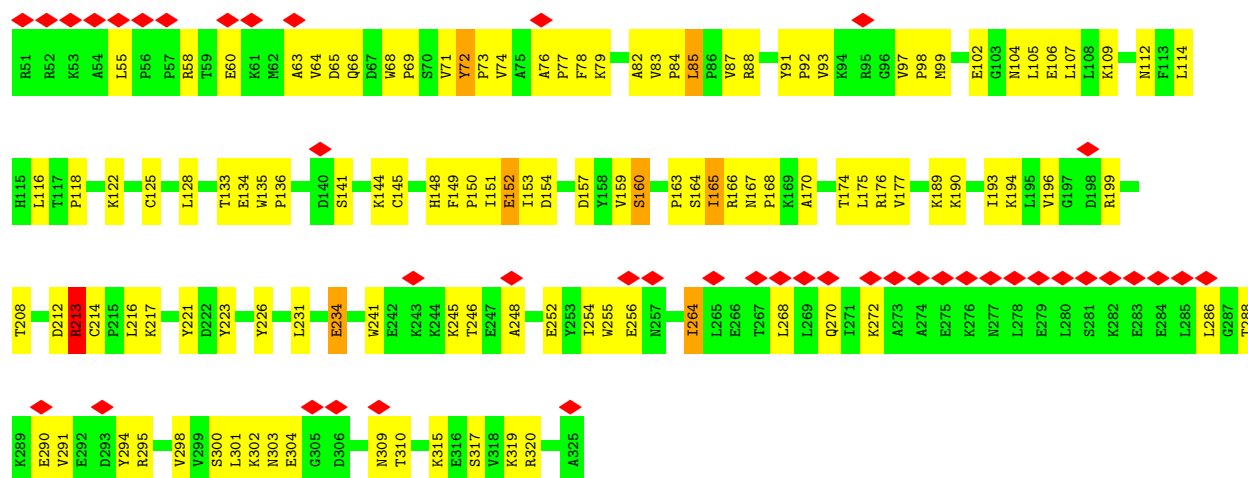


- Molecule 28: MITORIBOSOMAL PROTEIN MS34, MRPS34

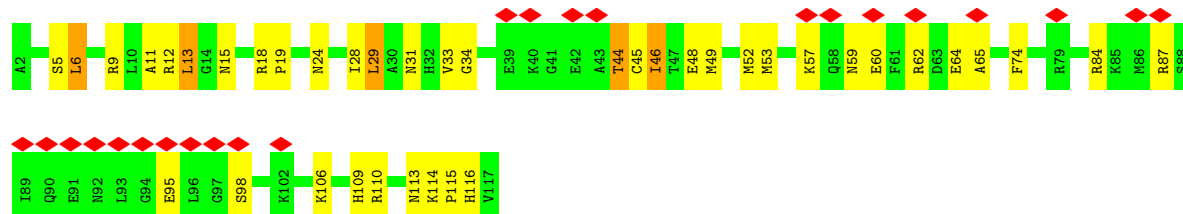


- Molecule 29: MITORIBOSOMAL PROTEIN MS35, MRPS35

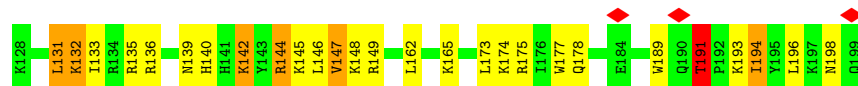




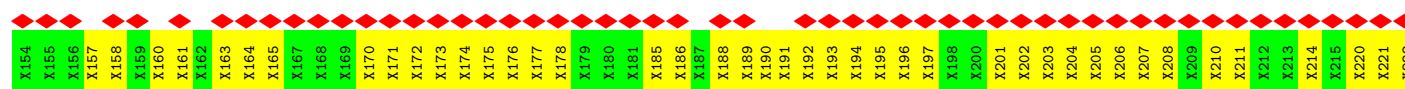
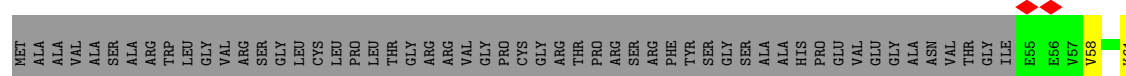
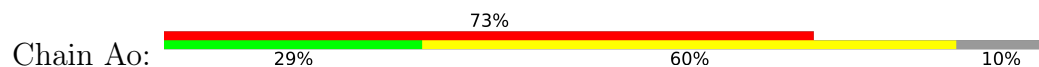
• Molecule 30: MITORIBOSOMAL PROTEIN MS37, MRPS37



• Molecule 31: MITORIBOSOMAL PROTEIN MS38, MRPS38

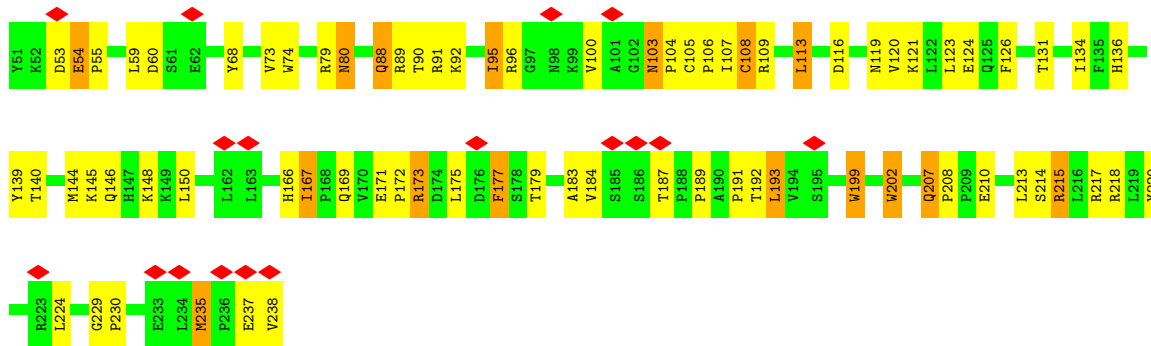


• Molecule 32: MITORIBOSOMAL PROTEIN MS39, MRPS39

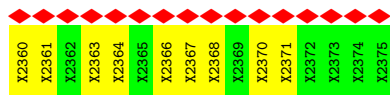




• Molecule 33: 28S RIBOSOMAL PROTEIN S18B, MITOCHONDRIAL

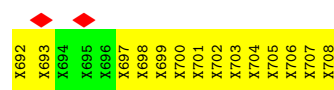


• Molecule 34: UNASSIGNED HELICES

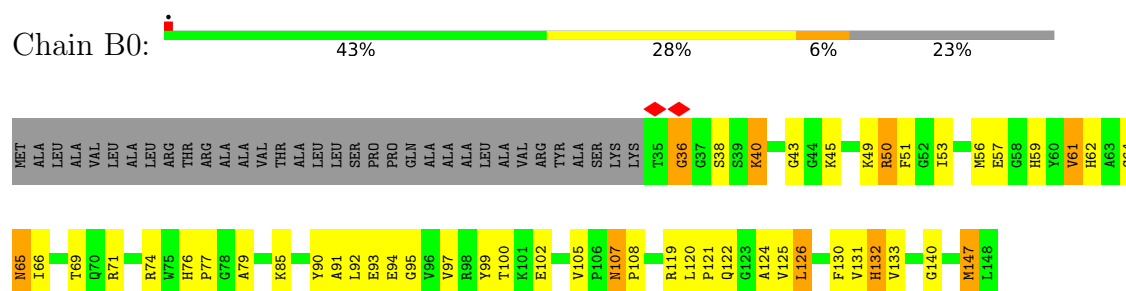


• Molecule 35: UNASSIGNED HELICES

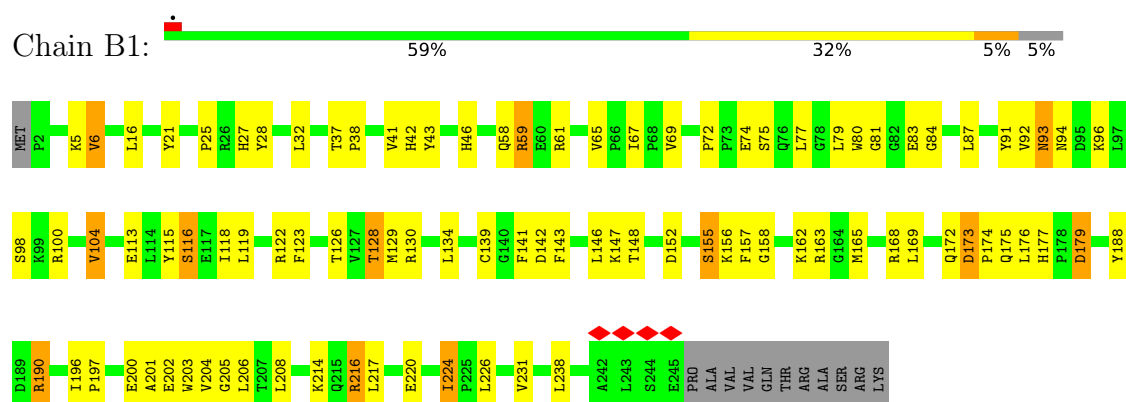




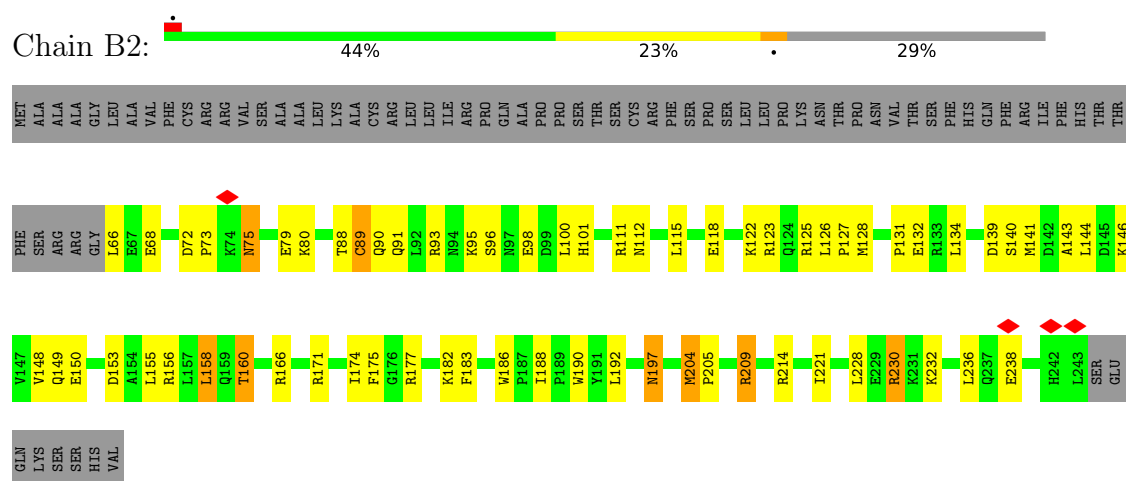
• Molecule 36: MITORIBOSOMAL PROTEIN BL27M, MRPL27



• Molecule 37: MITORIBOSOMAL PROTEIN BL28M, MRPL28

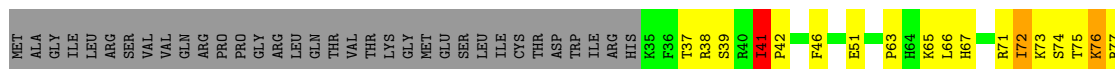


• Molecule 38: MITORIBOSOMAL PROTEIN UL29M, MRPL47

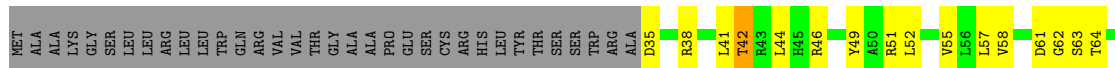


• Molecule 39: MITORIBOSOMAL PROTEIN UL30M, MRPL30

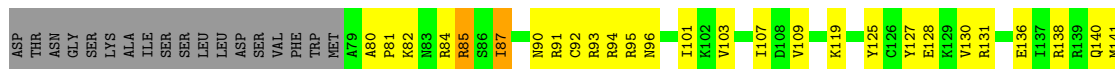
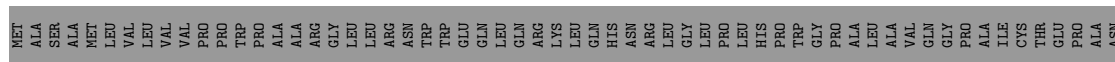




• Molecule 40: MITORIBOSOMAL PROTEIN BL31M, MRPL55



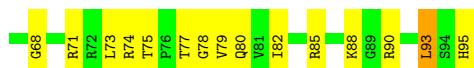
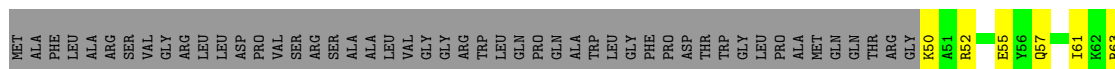
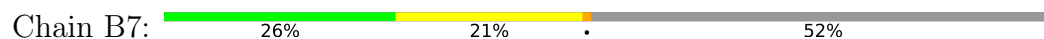
• Molecule 41: MITORIBOSOMAL PROTEIN BL32M, MRPL32



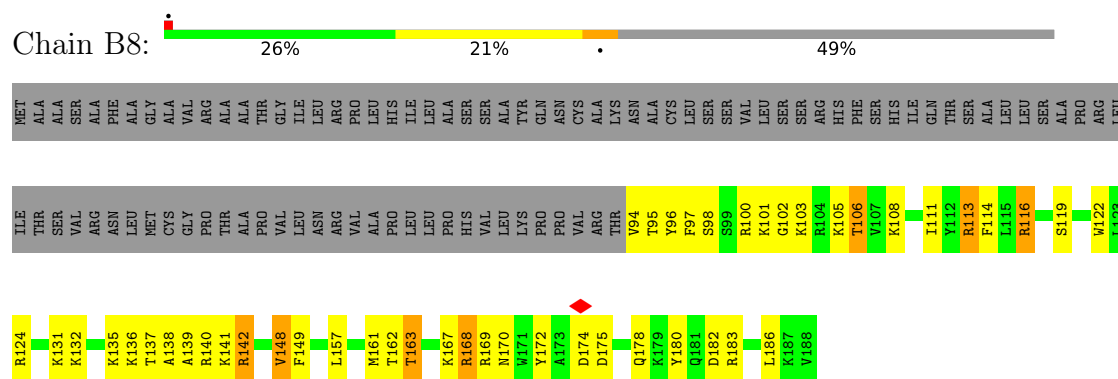
• Molecule 42: MITORIBOSOMAL PROTEIN BL33M, MRPL33



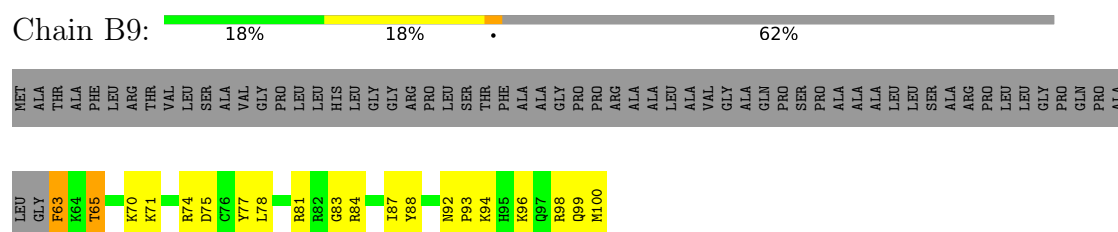
• Molecule 43: MITORIBOSOMAL PROTEIN BL34M, MRPL34



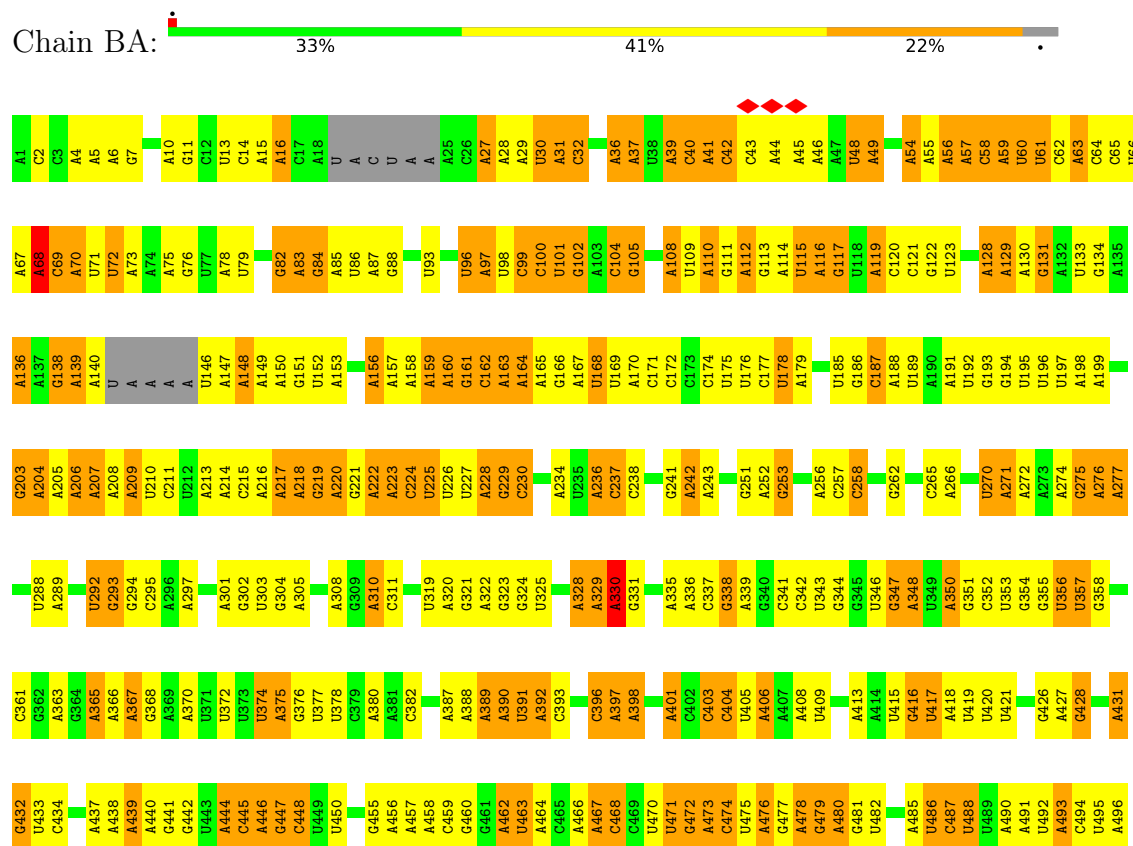
• Molecule 44: MITORIBOSOMAL PROTEIN BL35M, MRPL35



• Molecule 45: MITORIBOSOMAL PROTEIN BL36M, MRPL36



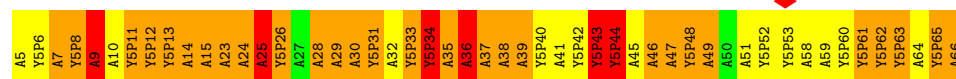
• Molecule 46: MITORIBOSOMAL 16S Ribosomal RNA



C1501	A1423	G1354	U1284	U1210	U1141	A1074	U1004	U853	A780	A704	U631	A560	C497
A1502	G1424	C1355	G1285	A1211	U1142	A1075	G1005	U856	A781	A705	G632	U561	C498
G1503	U1425	G1356	U1286	A	C1143	C	A1006	U857	C706	A707	A638	A562	A499
A1506	G1426	C1357	U1289	C	U1144	A1078	A1007	A858	U785	C710	U639	A563	U500
U1507	G1427	U1357	A1290	A	U1147	C1081	U1009	U859	A786	A711	G640	C565	G502
A1508	U1428	U1360	G1291	U	G1148	C1082	U1010	U862	C790	A714	A641	C566	U503
A1509	U1430	U1361	A1292	A	G1149	G1087	A1011	U866	A791	A715	G642	C567	A504
U1510	U1431	A1362	G1293	C	U1150	U1088	C1013	U870	A792	A716	A648	A568	G506
U1511	U1432	A1363	U1294	A	U1151	U1089	C1014	U871	G793	C717	C507	A570	C507
A1512	U1433	A1364	U1295	A1220	A1154	A	U1015	A870	U794	C718	A572	A571	C508
U1516	U1434	U1365	C1296	U1221	C1155	A	U1016	U871	C719	A719	C573	A510	U509
U1517	A1435	C1368	C1297	C1224	G1156	A	U1017	U875	A797	A720	C574	A511	A510
U1518	U1436	C1369	U1298	U1225	U1157	A	C1018	U876	A798	A721	U574	A512	A512
U1519	C1437	A1299	A1299	U1226	C1158	C	C1019	U877	G799	A722	U575	A513	A513
A1520	U1438	U1300	A1227	A1227	C1159	A	G1020	C877	G800	A723	U576	A514	G514
A1521	U1439	C1301	U1228	U1228	A1160	C	U1021	C878	A801	A724	U577	A515	C515
U1522	U1440	G1302	U1229	U1229	A1161	C	G1022	C879	A802	A725	U578	A516	A516
C1523	U1443	U1305	G1230	G1230	G1162	U	A1023	A880	C805	C726	U579	A517	G517
U1524	A1446	A1306	A1231	A1231	U1163	C	A1024	A881	G806	A732	C580	C518	C518
A1526	U1449	U1307	U1232	U1232	C1165	C	G1025	U882	A807	A733	A581	C519	C519
C1527	U1450	A1308	C1233	C1233	A1166	C	A1026	G883	C808	A734	A582	A583	A520
A1528	U1451	G1309	A1236	A1236	A1167	A	G1030	C885	A809	C735	C584	U521	C522
C1529	U1452	U1312	A1237	A1237	A1170	C	G1031	A886	C812	U736	C587	A523	A523
U1530	C1453	U1313	A1238	A1238	A1171	A	A1032	C	A813	U737	U588	A524	A524
A1532	U1454	U1314	U1239	U1239	C1176	A	G1033	C	U738	U738	U589	U525	U525
U1533	C1455	A1315	U1240	U1240	G1177	G	U1034	A889	A816	U741	G590	U526	U526
U1534	U1456	U1319	U1241	U1241	U1178	G	U1035	G890	A817	A742	C591	A527	A527
A1535	U1457	C1319	U1242	U1242	A1179	G	A1036	U891	C818	A743	C592	A528	A528
U1541	U1465	C1322	G1243	G1243	G1180	A	A1037	U892	C819	A744	C593	G529	G529
A1542	A1466	G1323	U1244	U1244	U1181	U	A1038	U893	G822	U745	A594	A530	A530
A1543	U1471	A1324	C1246	C1246	G1182	A	A1039	A894	G823	U746	U677	A531	A531
A1546	U1472	U1325	A1247	A1247	A1183	A	U1043	C896	C826	A747	U679	C598	C598
A1547	A1473	G1326	U1248	U1248	U1184	A	A1044	C897	U827	A748	U680	G600	G600
U1548	U1474	U1327	G1249	G1249	U1185	A	U1045	C898	U828	U749	U681	A602	A602
C1549	U1475	U1328	G1250	G1250	U1186	C	C1048	C900	U829	U750	C683	C603	A539
A1550	U1476	G1330	G1251	G1251	A1187	U	A1049	G904	C831	A751	U685	U611	C542
A1551	G1477	A1334	A1254	A1254	A1188	A	A1050	U905	C832	A755	A686	U611	C543
G1552	U1480	G1335	A1255	A1255	U1190	A	A1051	A906	A833	C761	U687	A615	A545
C1555	C1481	G1336	U1258	U1258	U1191	A	A1052	U	A834	A762	U688	A616	A546
A1557	U1482	A1337	U1259	U1259	U1192	C	A1053	U	C841	A763	A689	A617	C547
G1565	A1484	C1340	G1262	G1262	U1193	A	A1054	C909	C844	A767	A690	A618	A548
C1568	U1488	U1341	U1263	U1263	U1197	A	A1055	G911	C841	A768	U693	A619	A549
A1569	A1489	C1342	U1264	U1264	U1198	A	U1060	U991	C844	A772	C695	G621	U551
C1569	U1490	A1343	A1265	A1265	U1199	A	U1061	A992	U845	A773	U696	A622	U552
C1569	U1491	G1344	G1266	G1266	U1200	A	G1062	C993	U846	C774	G697	A623	C553
C1569	U1492	A1345	G1267	G1267	C1201	A	A1063	U994	U847	A775	A698	A624	A554
C1569	U1493	A1415	A1346	A1346	U1202	A	G1065	U995	C849	A776	C625	A626	C555
C1569	U1494	U1347	A1269	A1269	U1204	A	U1069	C914	C850	A777	A701	A629	C556
C1569	U1495	G1348	C1276	C1276	C1205	A	A1070	A999	A851	A778	U702	A630	A558
C1569	U1496	U1349	A1280	A1280	A1206	A	U1071	A1002	U852	A779	U703		
C1569	U1497	A1351	A1281	A1281	A1209	A	U1073	G926					

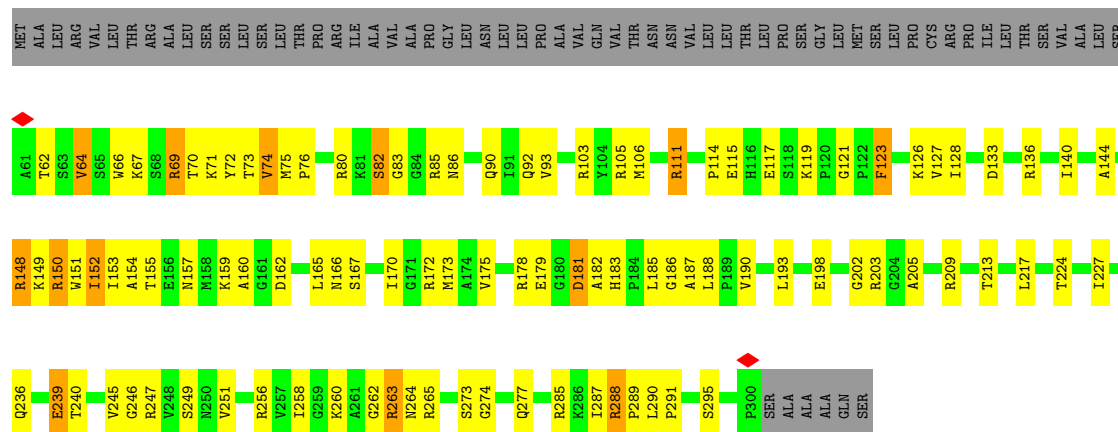
- Molecule 47: MITORIBOSOMAL CP TRNA

Chain BB: 29% 55% 12%



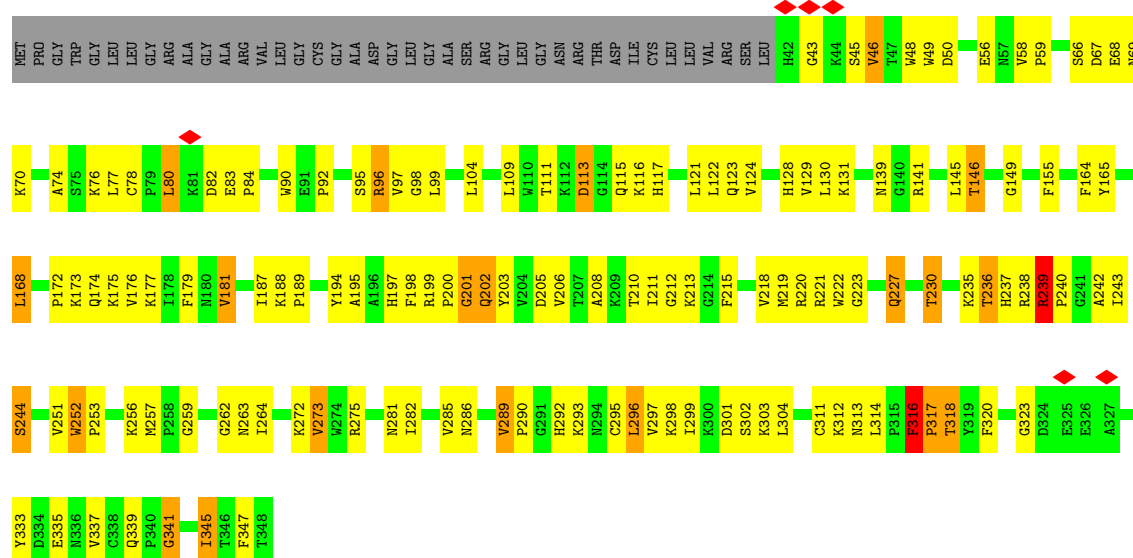
- Molecule 48: MITORIBOSOMAL PROTEIN UL2M, MRPL2

Chain BD: 45% 29% 22%



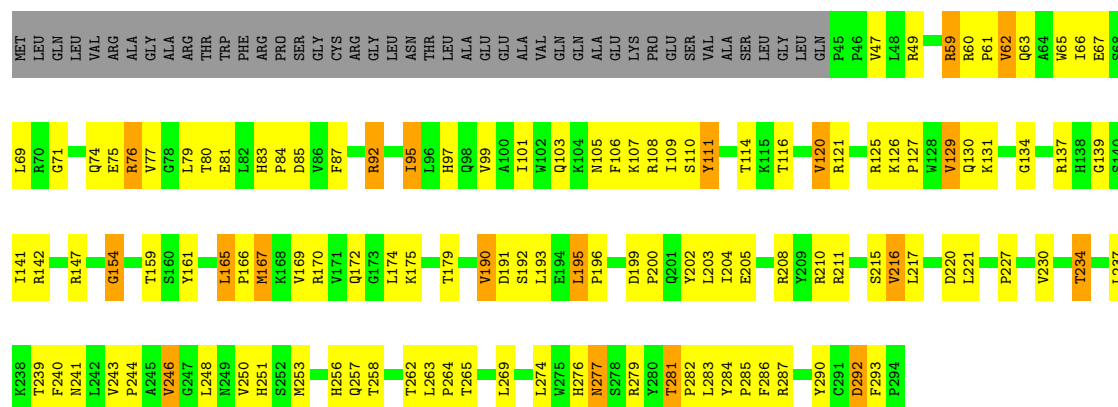
- Molecule 49: MITORIBOSOMAL PROTEIN UL3M, MRPL3

Chain BE: 47% 34% 6% 12%

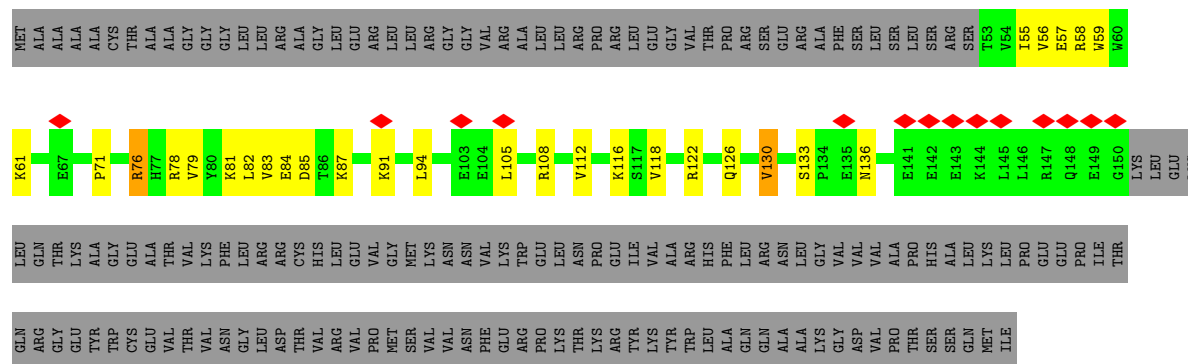


- Molecule 50: MITORIBOSOMAL PROTEIN UL4M, MRPL4

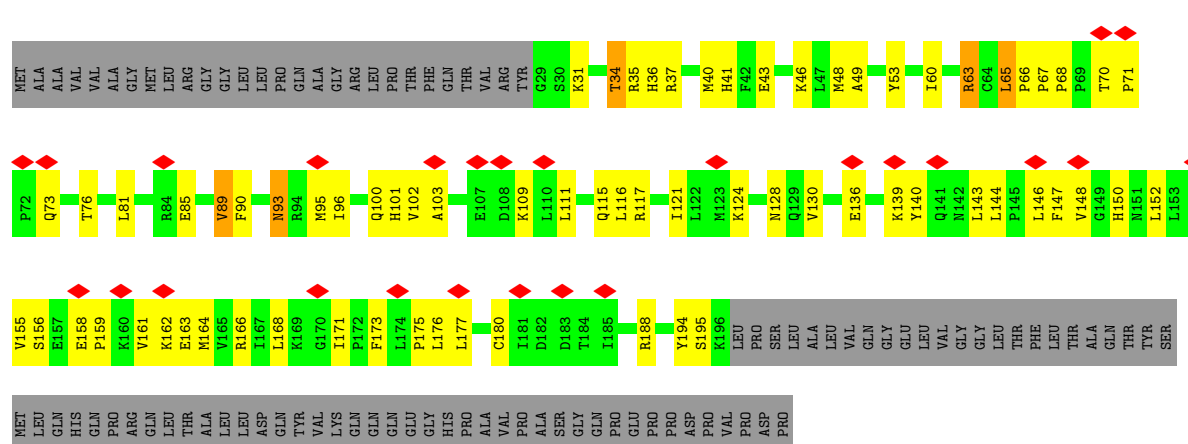
Chain BF: 44% 34% 6% 15%



• Molecule 51: MITORIBOSOMAL PROTEIN BL9M, MRPL9

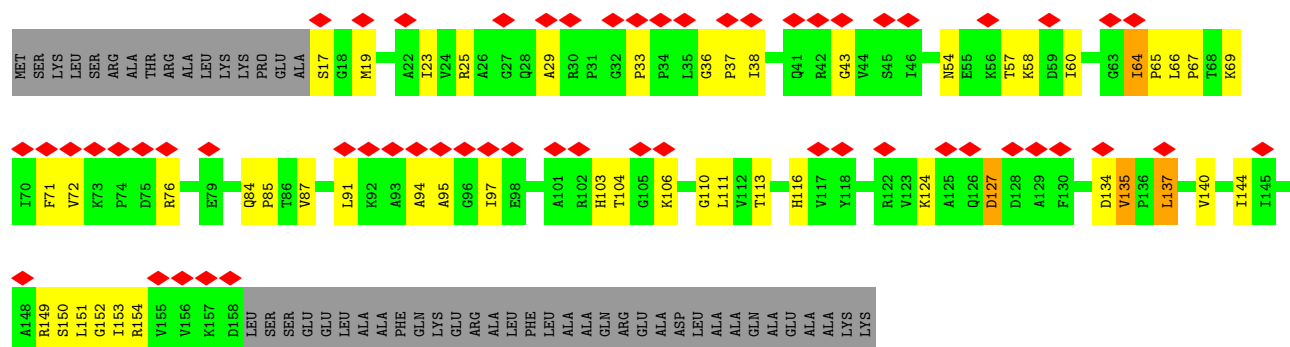


• Molecule 52: MITORIBOSOMAL PROTEIN UL10M, MRPL10



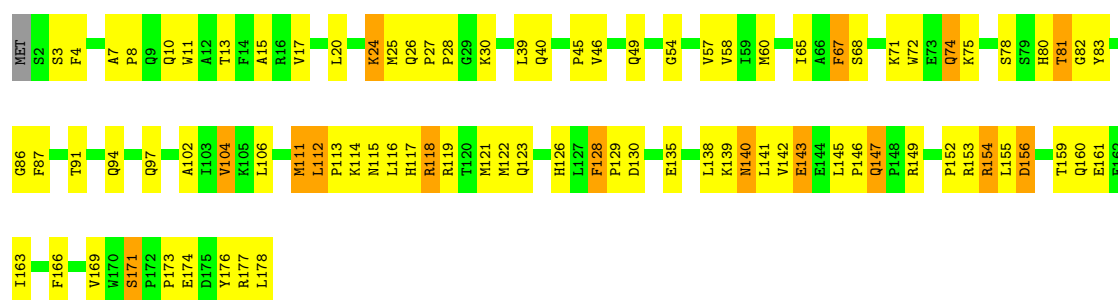
• Molecule 53: MITORIBOSOMAL PROTEIN UL11M, MRPL11





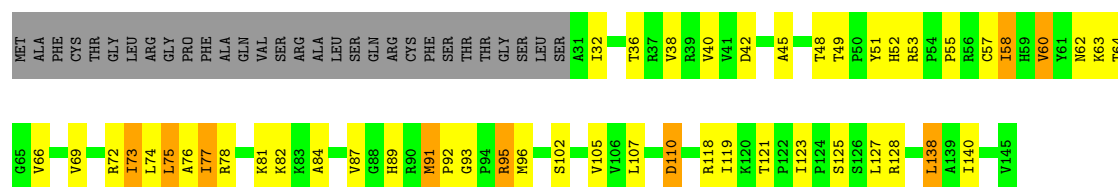
• Molecule 54: MITORIBOSOMAL PROTEIN UL13M, MRPL13

Chain BN: 49% 42% 8% .



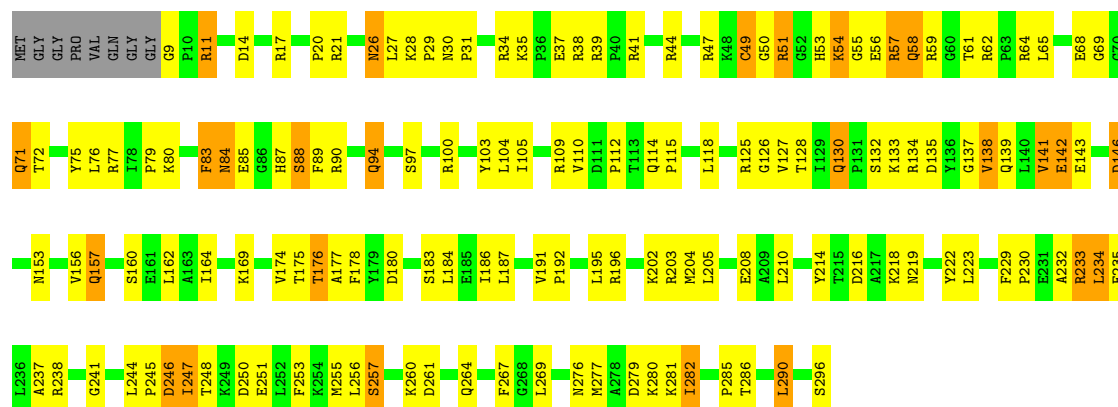
• Molecule 55: MITORIBOSOMAL PROTEIN UL14M, MRPL14

Chain BO: 45% 28% 6% 21%

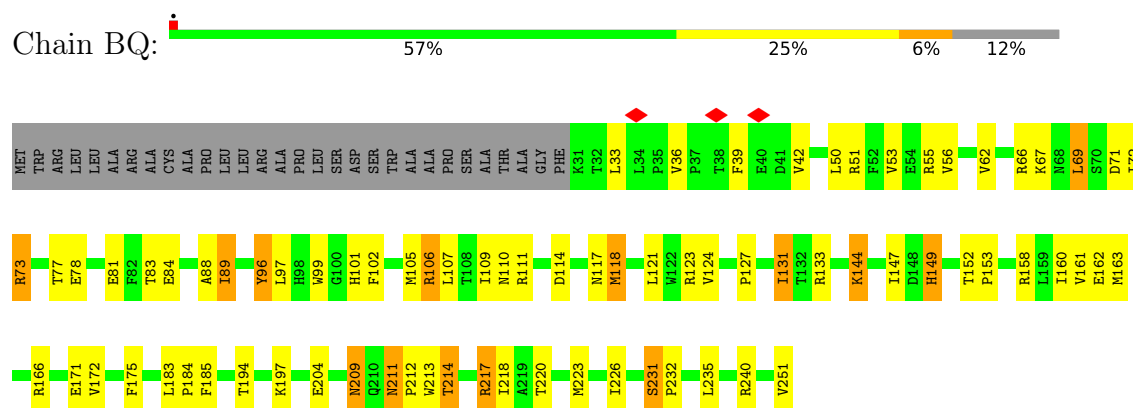


• Molecule 56: MITORIBOSOMAL PROTEIN UL15M, MRPL15

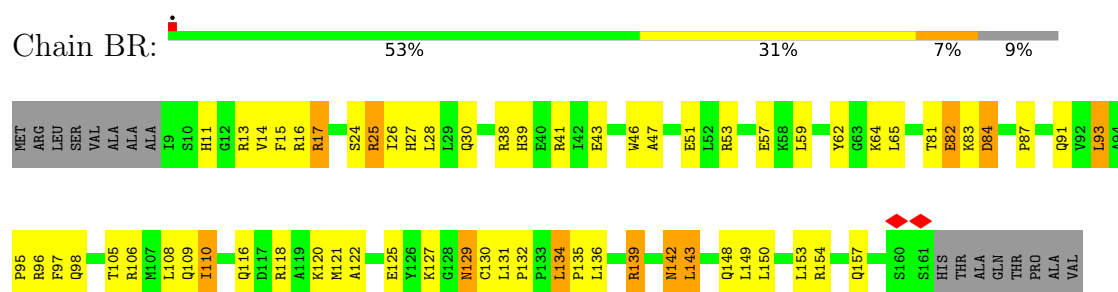
Chain BP: 48% 41% 9% .



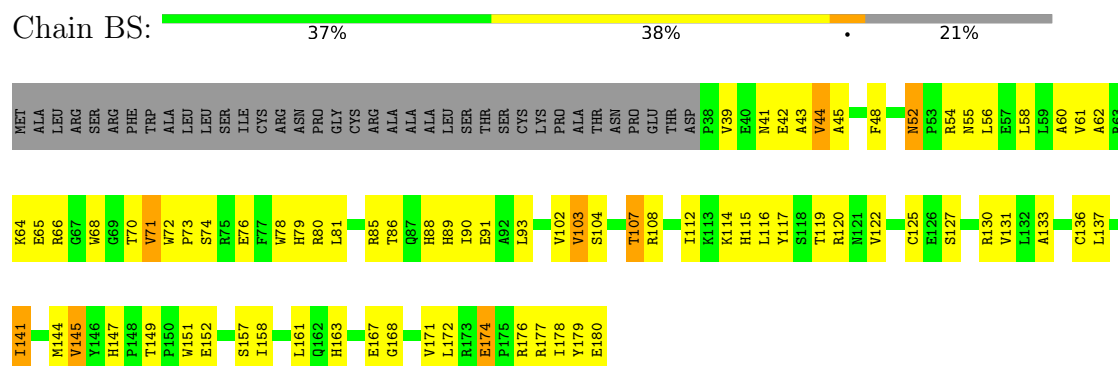
• Molecule 57: MITORIBOSOMAL PROTEIN UL16M, MRPL16



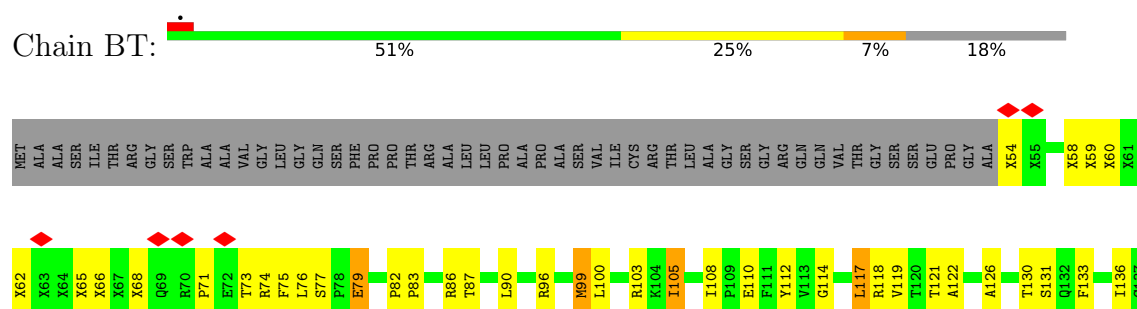
• Molecule 58: MITORIBOSOMAL PROTEIN BL17M, MRPL17

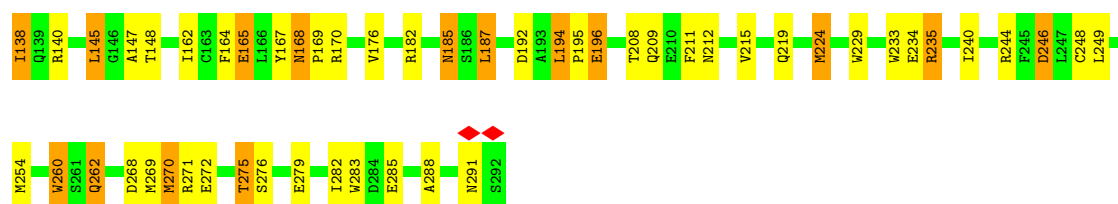


• Molecule 59: MITORIBOSOMAL PROTEIN UL18M, MRPL18

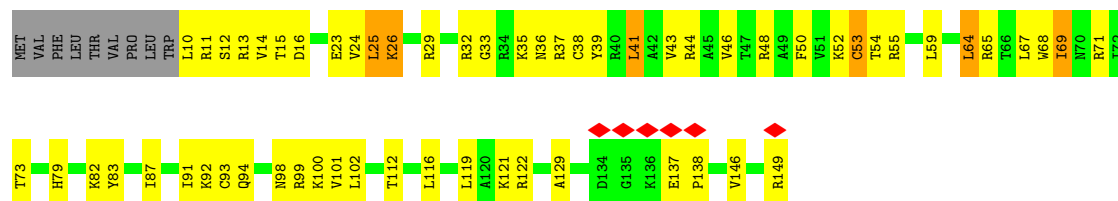


• Molecule 60: MITORIBOSOMAL PROTEIN BL19M, MRPL19

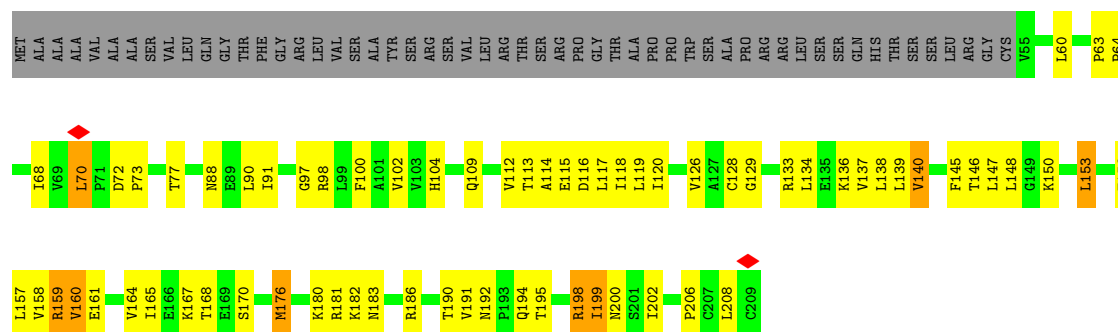




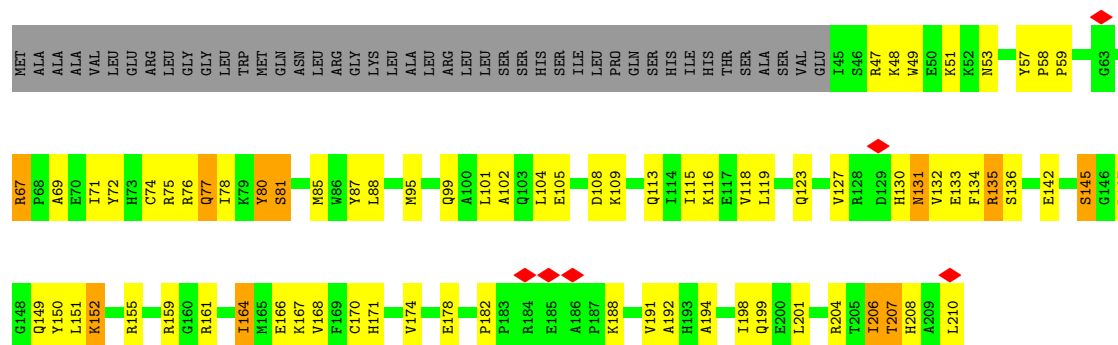
• Molecule 61: MITORIBOSOMAL PROTEIN BL20M, MRPL20



• Molecule 62: MITORIBOSOMAL PROTEIN BL21M, MRPL21

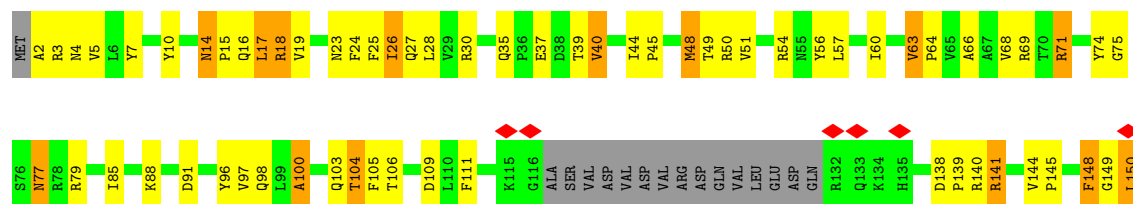


• Molecule 63: MITORIBOSOMAL PROTEIN UL22M, MRPL22

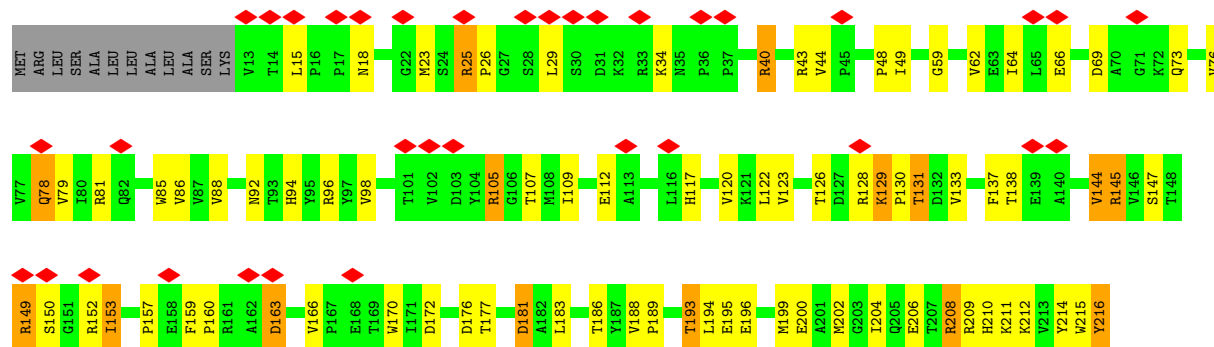


• Molecule 64: MITORIBOSOMAL PROTEIN UL23M, MRPL23

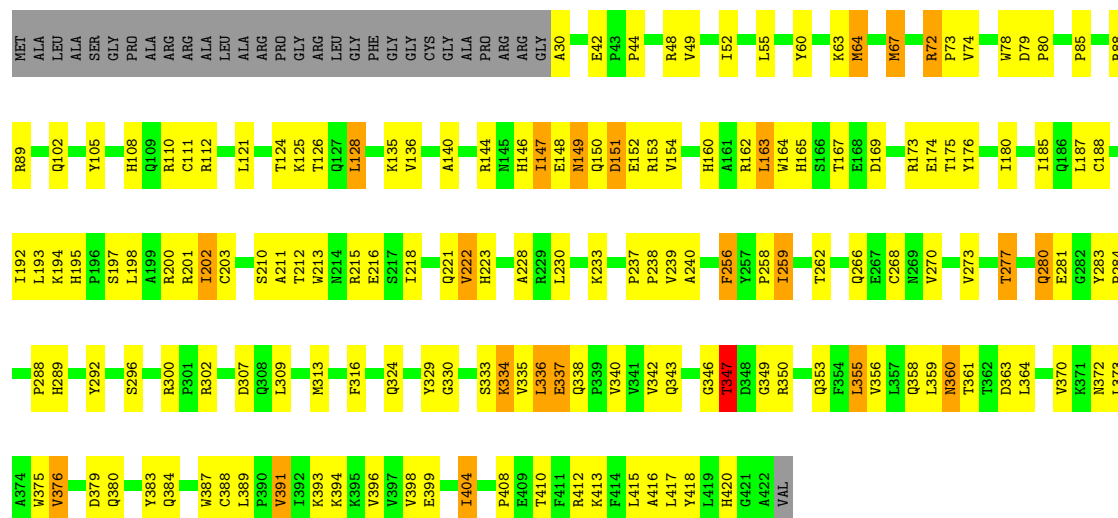




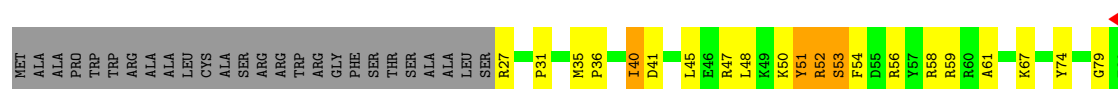
• Molecule 65: MITORIBOSOMAL PROTEIN UL24M, MRPL24

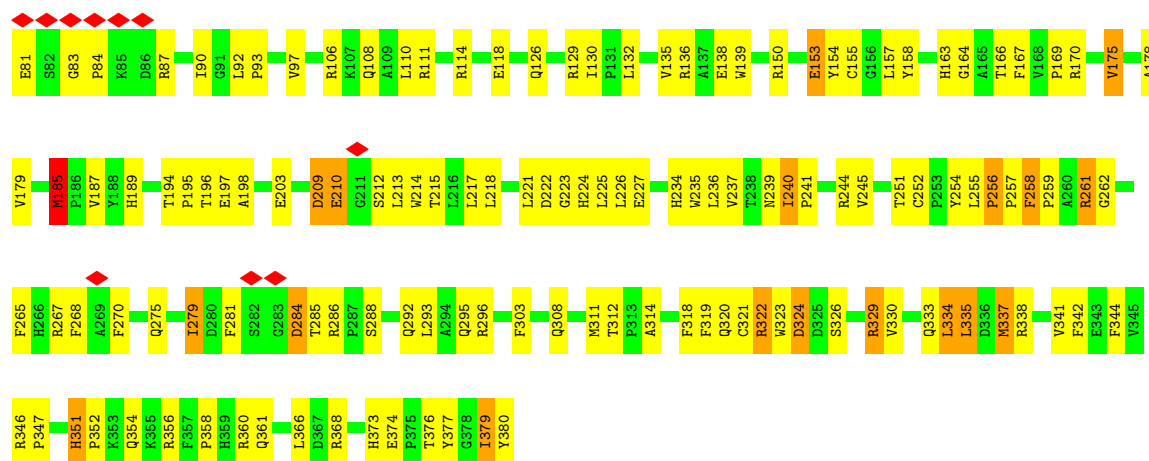


• Molecule 66: MITORIBOSOMAL PROTEIN ML37, MRPL37

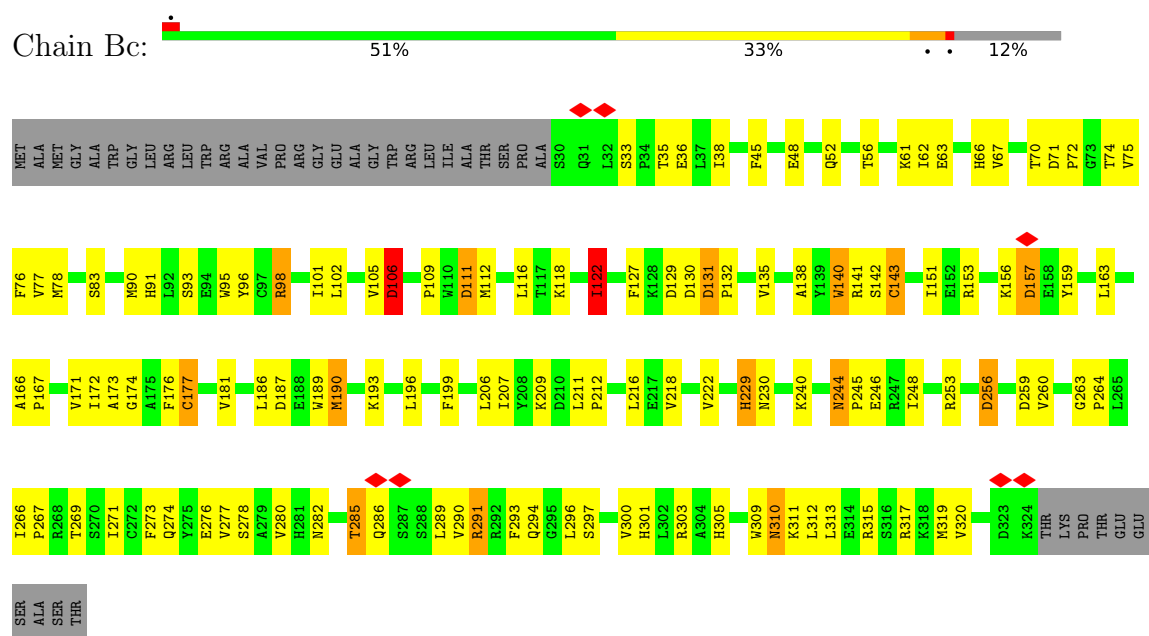


• Molecule 67: MITORIBOSOMAL PROTEIN ML38, MRPL38

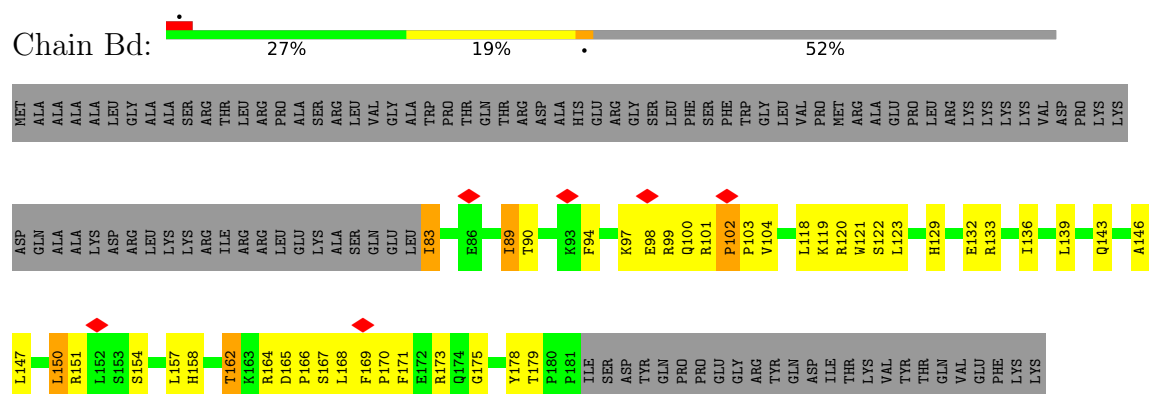




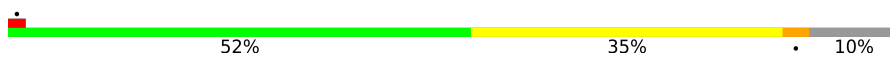
• Molecule 68: MITORIBOSOMAL PROTEIN ML39, MRPL39

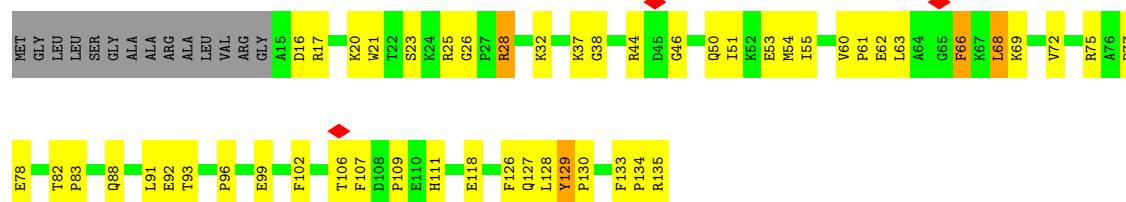


• Molecule 69: MITORIBOSOMAL PROTEIN ML40, MRPL40

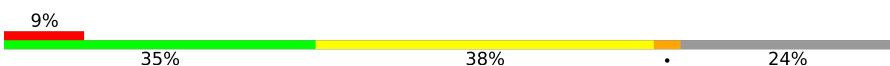


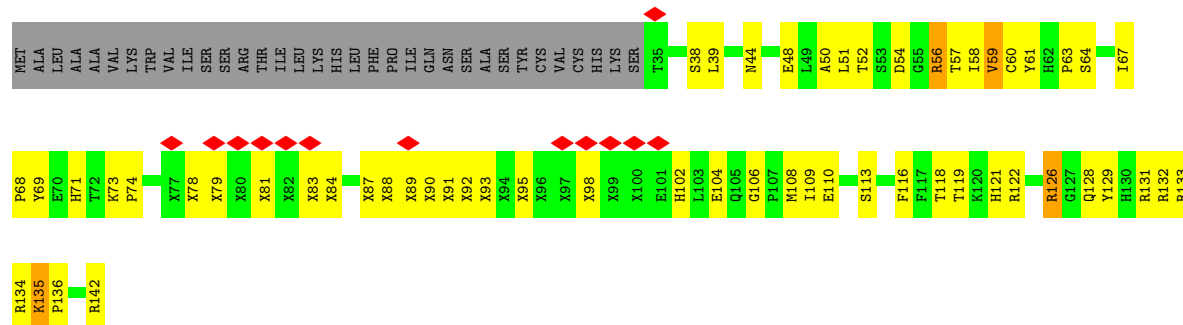
• Molecule 70: MITORIBOSOMAL PROTEIN ML41, MRPL41

Chain Be: 



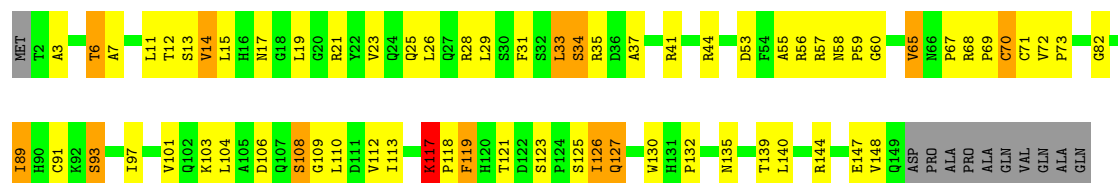
- Molecule 71: MITORIBOSOMAL PROTEIN ML42, MRPL42

Chain Bf: 



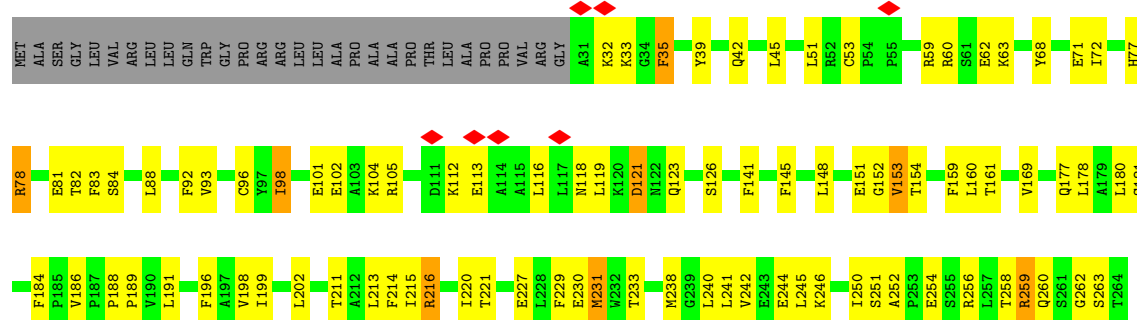
- Molecule 72: MITORIBOSOMAL PROTEIN ML43, MRPL43

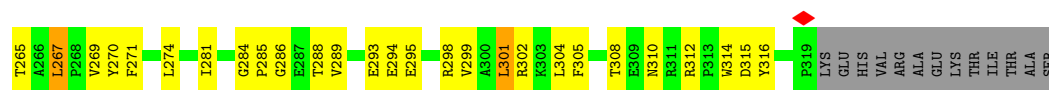
Chain Bg: 



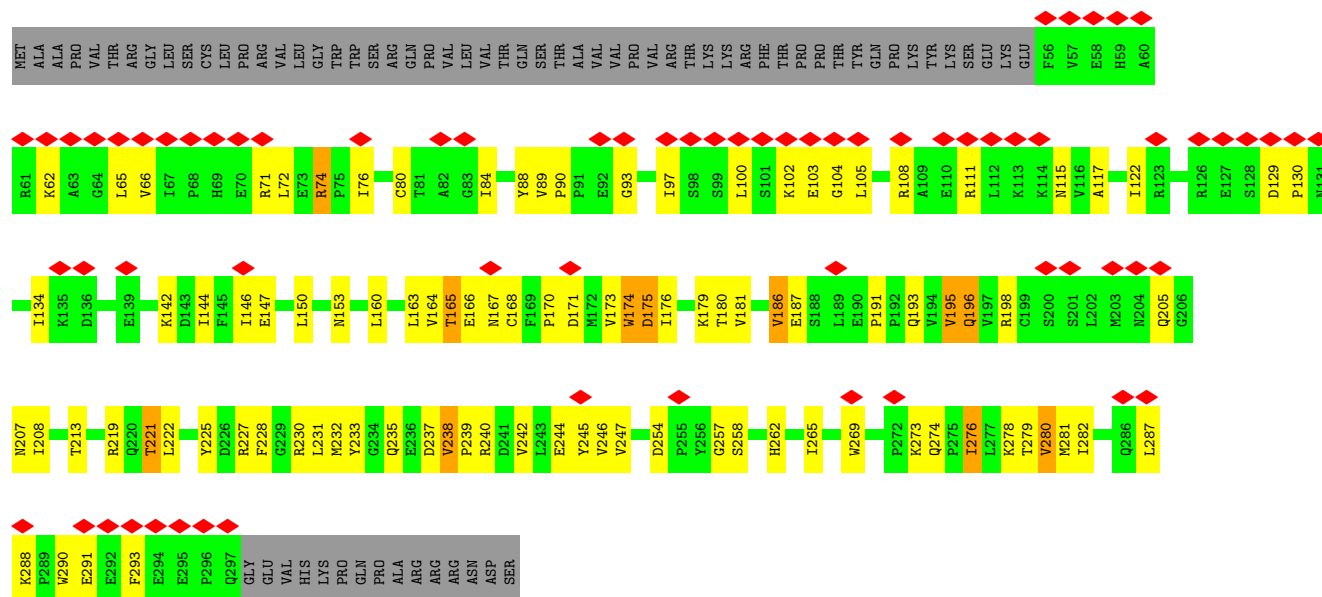
- Molecule 73: MITORIBOSOMAL PROTEIN ML44, MRPL44

Chain Bh: 

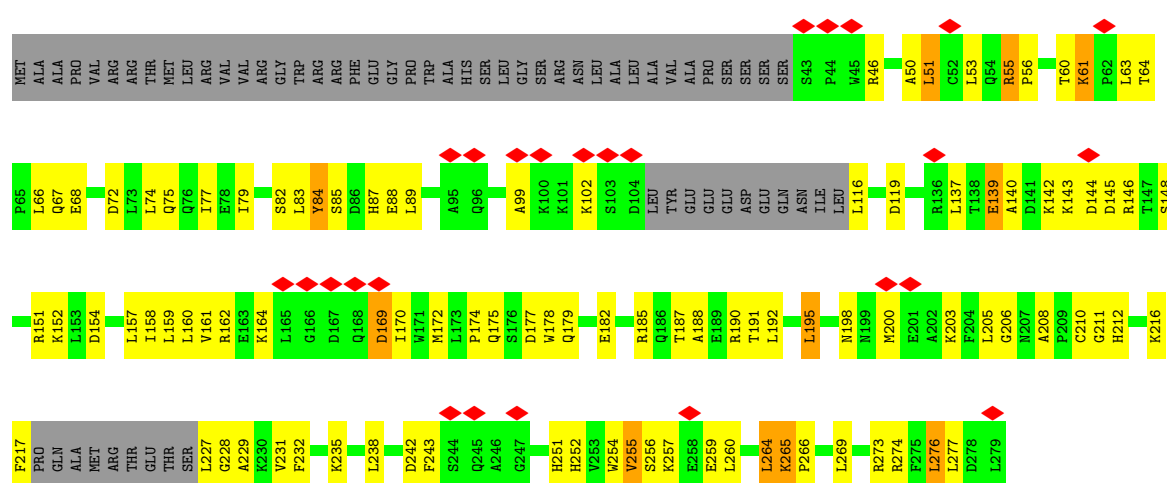
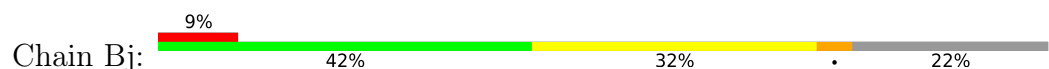




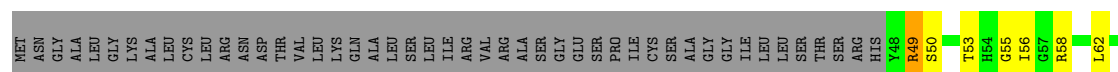
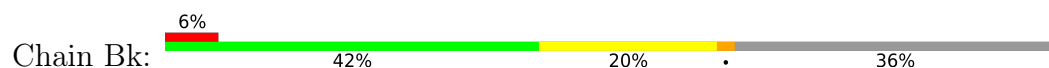
• Molecule 74: MITORIBOSOMAL PROTEIN ML45, MRPL45

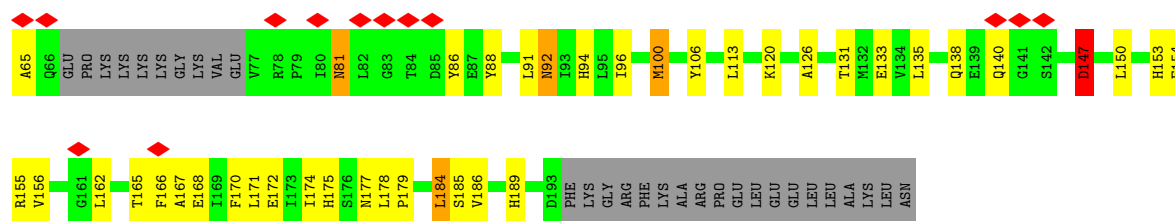


• Molecule 75: MITORIBOSOMAL PROTEIN ML46, MRPL46

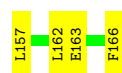
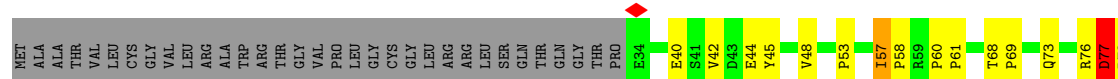


• Molecule 76: MITORIBOSOMAL PROTEIN ML48, MRPL48

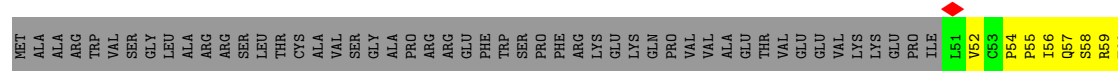




• Molecule 77: MITORIBOSOMAL PROTEIN ML49, MRPL49



• Molecule 78: MITORIBOSOMAL PROTEIN ML50, MRPL50

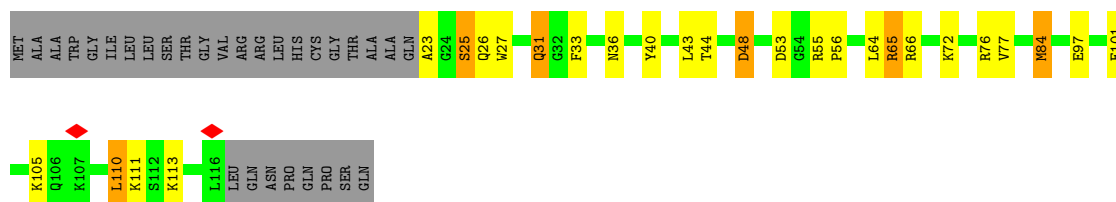


• Molecule 79: MITORIBOSOMAL PROTEIN ML51, MRPL51

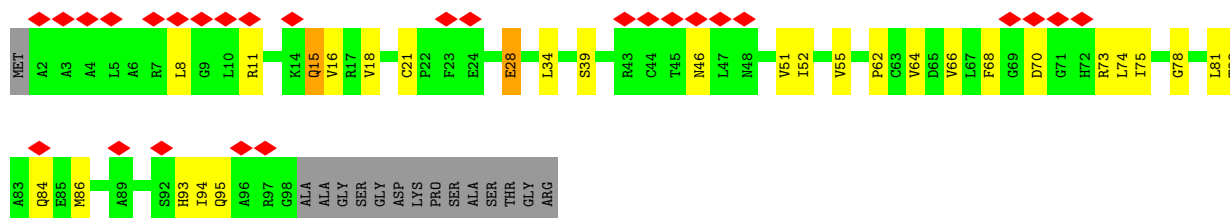


• Molecule 80: MITORIBOSOMAL PROTEIN ML52, MRPL52

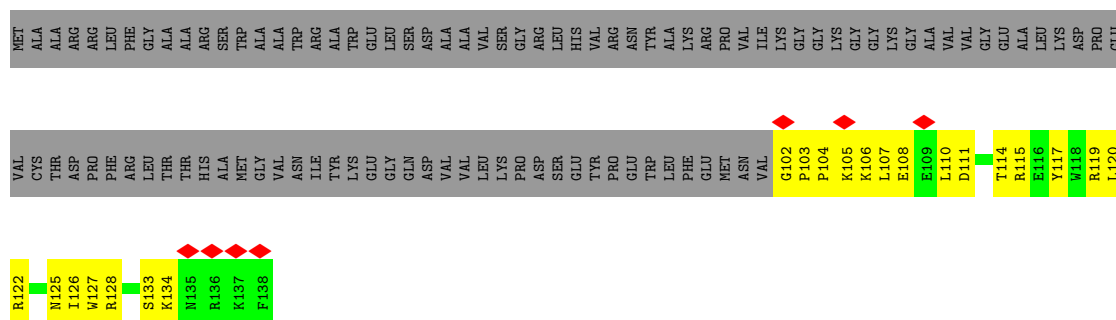




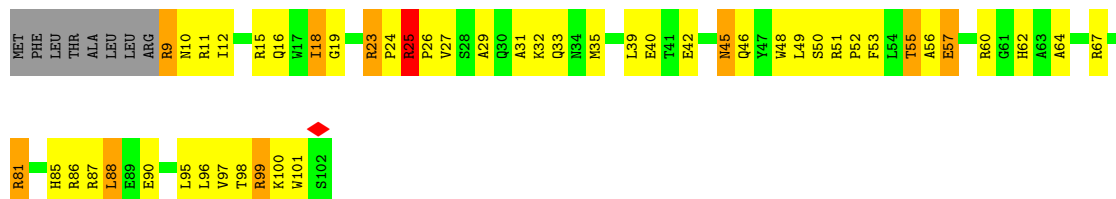
• Molecule 81: MITORIBOSOMAL PROTEIN ML53, MRPL53



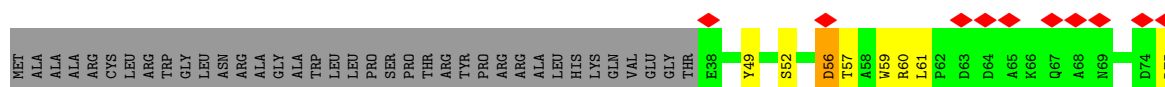
• Molecule 82: MITORIBOSOMAL PROTEIN ML54, MRPL54

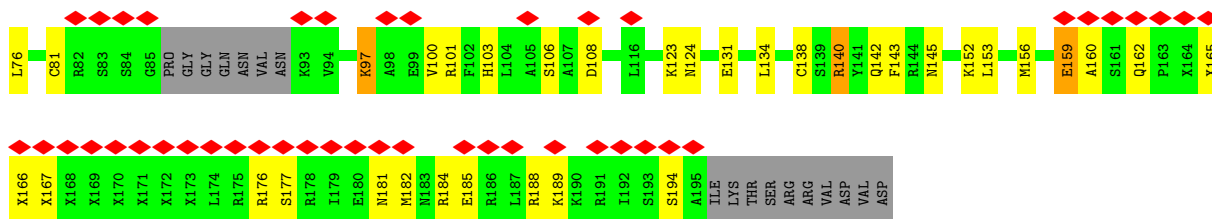


• Molecule 83: MITORIBOSOMAL PROTEIN ML63, MRPL57

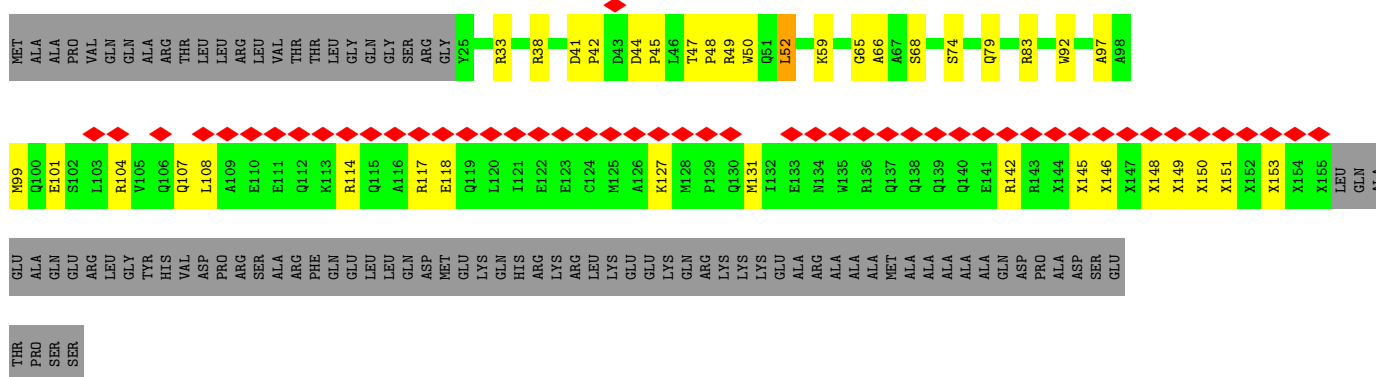
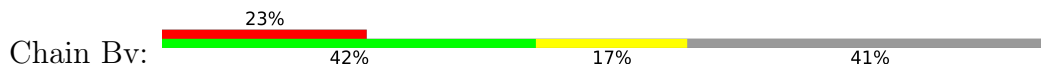


• Molecule 84: MITORIBOSOMAL PROTEIN ML62, MRPL58

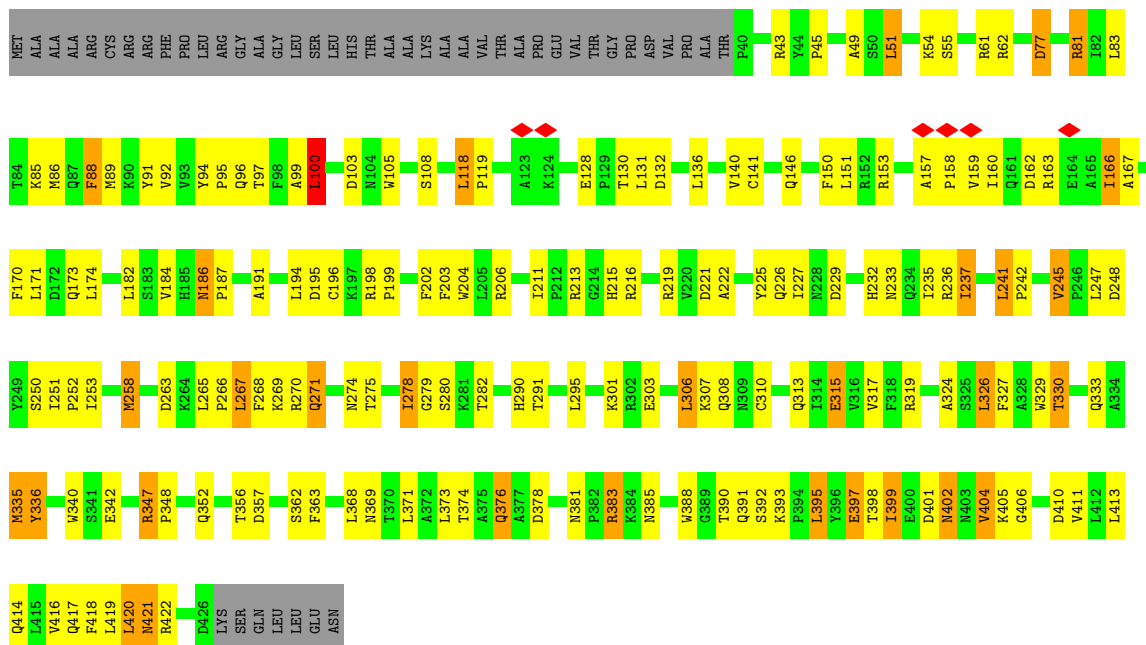




• Molecule 85: MITORIBOSOMAL PROTEIN ML64, MRPL59

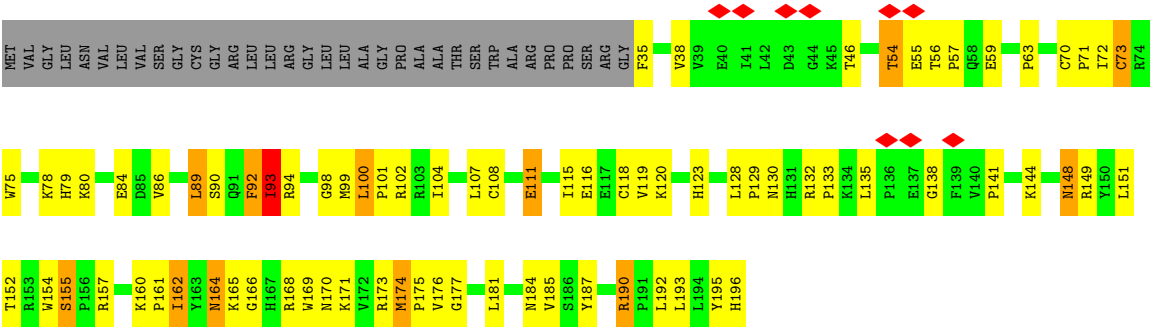


• Molecule 86: MITORIBOSOMAL PROTEIN ML65, MRPS30

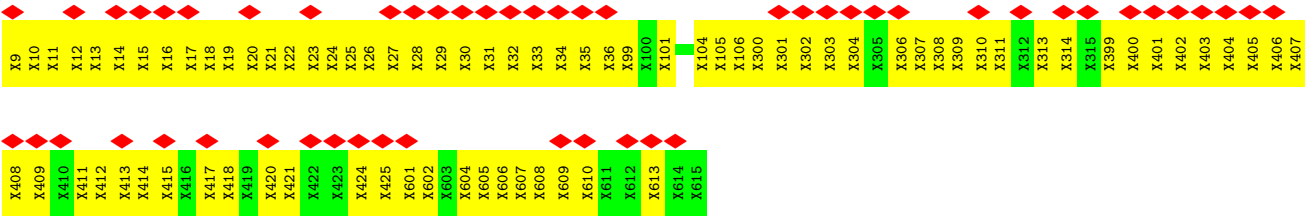


• Molecule 87: MITORIBOSOMAL PROTEIN ML66, MRPS18A





● Molecule 88: UNASSIGNED SECONDARY STRUCTURE ELEMENTS



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	60872	Depositor
Resolution determination method	Not provided	
CTF correction method	PER DETECTOR FRAME	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: Y5P, ZN, MG, GDP, P5P

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.25	0/22852	0.41	0/35580
2	AB	0.47	0/1804	0.88	5/2445 (0.2%)
3	AC	0.44	0/1105	0.93	5/1496 (0.3%)
4	AE	0.43	0/2673	0.84	2/3591 (0.1%)
5	AF	0.48	0/1008	0.99	5/1358 (0.4%)
6	AG	0.46	0/1763	0.85	4/2368 (0.2%)
7	AI	0.44	1/2455 (0.0%)	0.82	5/3291 (0.2%)
8	AJ	0.47	0/1091	0.93	2/1474 (0.1%)
9	AK	0.51	0/1021	1.01	3/1381 (0.2%)
10	AL	0.42	0/858	0.97	5/1152 (0.4%)
11	AN	0.40	0/874	0.79	0/1171
12	AO	0.47	0/1473	0.93	6/1970 (0.3%)
13	AP	0.47	0/954	0.86	5/1284 (0.4%)
14	AQ	0.46	0/871	1.01	3/1181 (0.3%)
15	AR	0.51	0/802	0.93	5/1079 (0.5%)
16	AU	0.46	0/745	0.88	2/993 (0.2%)
19	Aa	0.46	0/2052	0.76	0/2774
20	Ab	0.42	0/1126	0.88	2/1514 (0.1%)
21	Ac	0.42	0/1399	0.94	4/1881 (0.2%)
22	Ad	0.46	0/1490	0.80	2/2005 (0.1%)
24	Af	0.38	0/790	0.86	2/1064 (0.2%)
25	Ag	0.47	0/2731	0.83	0/3696
26	Ah	0.38	0/903	0.85	3/1215 (0.2%)
27	Ai	0.39	0/841	0.81	0/1121
28	Aj	0.44	0/1779	0.91	7/2404 (0.3%)
29	Ak	0.44	0/2268	0.91	3/3069 (0.1%)
30	Am	0.48	0/947	0.90	2/1268 (0.2%)
31	An	0.53	0/650	0.90	2/858 (0.2%)
32	Ao	0.43	0/726	0.95	4/988 (0.4%)
33	Ap	0.46	0/1602	1.00	11/2175 (0.5%)
36	B0	0.70	0/901	1.10	7/1217 (0.6%)
37	B1	0.49	0/2093	0.88	3/2835 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	B2	0.52	0/1582	0.87	0/2118
39	B3	0.61	0/993	1.15	8/1341 (0.6%)
40	B4	0.37	0/388	1.08	3/523 (0.6%)
41	B5	0.56	0/917	0.96	5/1227 (0.4%)
42	B6	0.47	0/396	1.05	2/526 (0.4%)
43	B7	0.80	0/395	0.98	2/524 (0.4%)
44	B8	0.69	0/853	1.00	3/1136 (0.3%)
45	B9	0.70	0/342	0.87	0/450
46	BA	0.42	0/36094	0.56	4/56186 (0.0%)
48	BD	0.65	0/1898	1.06	10/2555 (0.4%)
49	BE	0.61	0/2493	1.09	17/3387 (0.5%)
50	BF	0.67	1/2069 (0.0%)	1.01	5/2816 (0.2%)
51	BI	0.50	0/819	0.87	0/1101
52	BJ	0.53	0/1392	1.01	8/1881 (0.4%)
53	BK	0.52	0/1099	0.92	4/1480 (0.3%)
54	BN	0.65	0/1487	1.05	11/2017 (0.5%)
55	BO	0.64	1/912 (0.1%)	0.97	1/1231 (0.1%)
56	BP	0.58	0/2368	1.03	8/3198 (0.3%)
57	BQ	0.60	0/1838	0.97	3/2475 (0.1%)
58	BR	0.59	0/1262	0.89	2/1700 (0.1%)
59	BS	0.52	0/1197	0.93	1/1624 (0.1%)
60	BT	0.55	0/1903	1.01	8/2567 (0.3%)
61	BU	0.72	0/1179	0.94	0/1578
62	BV	0.65	0/1256	1.01	2/1706 (0.1%)
63	BW	0.63	0/1407	0.95	2/1891 (0.1%)
64	BX	0.52	0/1149	1.05	5/1554 (0.3%)
65	BY	0.47	0/1704	0.96	6/2310 (0.3%)
66	Ba	0.52	0/3267	0.94	7/4455 (0.2%)
67	Bb	0.49	0/3047	0.97	10/4139 (0.2%)
68	Bc	0.45	0/2464	0.90	9/3330 (0.3%)
69	Bd	0.48	0/853	0.99	7/1153 (0.6%)
70	Be	0.52	0/996	1.01	5/1340 (0.4%)
71	Bf	0.51	0/731	1.00	2/990 (0.2%)
72	Bg	0.60	0/1191	1.08	8/1614 (0.5%)
73	Bh	0.52	0/2372	0.97	4/3211 (0.1%)
74	Bi	0.50	0/2034	0.90	5/2759 (0.2%)
75	Bj	0.43	0/1811	0.89	6/2436 (0.2%)
76	Bk	0.50	0/1108	0.96	1/1499 (0.1%)
77	Bl	0.56	0/1135	0.99	2/1549 (0.1%)
78	Bm	0.45	0/917	0.86	0/1248
79	Bn	0.71	0/860	1.06	4/1150 (0.3%)
80	Bo	0.57	0/762	0.93	1/1022 (0.1%)
81	Bp	0.49	0/752	0.95	3/1013 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
82	Bq	0.42	0/346	0.76	2/463 (0.4%)
83	Bt	0.63	0/798	1.20	5/1073 (0.5%)
84	Bu	0.45	0/1163	0.81	2/1557 (0.1%)
85	Bv	0.49	0/1022	0.78	1/1382 (0.1%)
86	Bw	0.57	0/3206	0.99	9/4354 (0.2%)
87	Bx	0.55	0/1364	1.04	7/1849 (0.4%)
All	All	0.47	3/166238 (0.0%)	0.80	329/236586 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
9	AK	0	1
49	BE	0	1
57	BQ	0	1
60	BT	0	1
67	Bb	0	2
79	Bn	0	1
83	Bt	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	BO	58	ILE	CA-CB	-6.02	1.49	1.55
7	AI	249	ILE	CA-C	5.87	1.56	1.52
50	BF	141	ILE	CA-CB	-5.48	1.47	1.54

The worst 5 of 329 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	Bt	23	ARG	CA-C-N	12.01	131.59	119.82
83	Bt	23	ARG	C-N-CA	12.01	131.59	119.82
73	Bh	284	GLY	CA-C-N	11.44	131.52	120.31
73	Bh	284	GLY	C-N-CA	11.44	131.52	120.31
12	AO	68	PRO	CA-C-N	10.22	130.91	120.38

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	AK	194	ARG	Peptide
49	BE	316	PHE	Peptide
57	BQ	149	HIS	Peptide
60	BT	275	THR	Peptide
67	Bb	164	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	20411	0	10345	375	0
2	AB	1762	0	1774	63	0
3	AC	1075	0	1087	48	0
4	AE	2621	0	2640	111	0
5	AF	990	0	1025	41	0
6	AG	1721	0	1747	53	0
7	AI	2498	0	2473	88	0
8	AJ	1067	0	1101	55	0
9	AK	1001	0	1037	42	0
10	AL	840	0	890	27	0
11	AN	858	0	883	46	0
12	AO	1448	0	1536	38	0
13	AP	932	0	951	43	0
14	AQ	853	0	913	46	0
15	AR	784	0	813	35	0
16	AU	734	0	745	32	0
17	AV	1251	0	823	72	0
17	AY	1251	0	824	77	0
18	AX	231	0	157	7	0
19	Aa	2296	0	2317	166	0
20	Ab	1101	0	1118	33	0
21	Ac	1367	0	1385	56	0
22	Ad	1467	0	1466	49	0
23	Ae	2016	0	2028	447	0
24	Af	778	0	791	34	0
25	Ag	2774	0	2810	146	0
26	Ah	876	0	832	32	0
27	Ai	824	0	842	32	0
28	Aj	1777	0	1788	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Ak	2222	0	2270	88	0
30	Am	930	0	959	32	0
31	An	639	0	709	26	0
32	Ao	3028	0	3081	437	0
33	Ap	1551	0	1519	72	0
34	As	96	0	98	11	0
35	Az	102	0	104	25	0
36	B0	878	0	896	40	0
37	B1	2036	0	2058	66	0
38	B2	1544	0	1580	64	0
39	B3	968	0	1018	40	0
40	B4	381	0	400	19	0
41	B5	902	0	916	38	0
42	B6	391	0	429	27	0
43	B7	387	0	413	15	0
44	B8	833	0	883	45	0
45	B9	335	0	359	17	0
46	BA	32233	0	16311	725	0
47	BB	1008	0	555	32	0
48	BD	1860	0	1923	73	0
49	BE	2420	0	2418	114	0
50	BF	2011	0	2049	103	0
51	BI	805	0	845	25	0
52	BJ	1361	0	1448	52	0
53	BK	1081	0	1146	38	0
54	BN	1444	0	1437	73	0
55	BO	896	0	946	39	0
56	BP	2312	0	2373	130	0
57	BQ	1792	0	1832	54	0
58	BR	1240	0	1260	52	0
59	BS	1168	0	1159	74	0
60	BT	1950	0	1969	72	0
61	BU	1159	0	1228	58	0
62	BV	1231	0	1278	55	0
63	BW	1374	0	1405	56	0
64	BX	1120	0	1133	68	0
65	BY	1663	0	1665	67	0
66	Ba	3173	0	3153	121	0
67	Bb	2952	0	2840	134	0
68	Bc	2408	0	2415	95	0
69	Bd	832	0	828	50	0
70	Be	968	0	968	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
71	Bf	852	0	834	69	0
72	Bg	1167	0	1173	63	0
73	Bh	2319	0	2332	93	0
74	Bi	1979	0	1974	83	0
75	Bj	1775	0	1797	78	0
76	Bk	1087	0	1080	47	0
77	Bl	1097	0	1080	32	0
78	Bm	893	0	878	37	0
79	Bn	837	0	860	42	0
80	Bo	747	0	748	23	0
81	Bp	742	0	749	18	0
82	Bq	336	0	342	21	0
83	Bt	780	0	792	47	0
84	Bu	1208	0	1227	40	0
85	Bv	1068	0	1032	29	0
86	Bw	3126	0	3153	132	0
87	Bx	1325	0	1354	75	0
88	Bz	564	0	574	131	0
89	AA	146	0	0	0	0
89	Ag	1	0	0	0	0
89	B0	1	0	0	0	0
89	B2	1	0	0	0	0
89	BA	195	0	0	0	0
89	BD	2	0	0	0	0
89	BE	1	0	0	0	0
89	BP	1	0	0	0	0
89	BR	2	0	0	0	0
89	BX	1	0	0	0	0
90	AR	1	0	0	0	0
90	Ac	1	0	0	0	0
90	Ap	1	0	0	0	0
90	B5	1	0	0	0	0
90	B9	1	0	0	0	0
90	Bx	1	0	0	0	0
91	Ag	28	0	12	0	0
92	AA	114	0	0	7	0
92	Ag	4	0	0	1	0
92	B0	3	0	0	0	0
92	B7	2	0	0	0	0
92	B8	1	0	0	0	0
92	BA	196	0	0	12	0
92	BD	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	BF	4	0	0	0	0
92	BI	1	0	0	0	0
92	BO	2	0	0	0	0
92	BP	3	0	0	2	0
92	BR	2	0	0	0	0
92	BU	1	0	0	0	0
92	BW	4	0	0	0	0
All	All	167915	0	141408	5789	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 5789 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Ao:558:UNK:HG1	32:Ao:576:UNK:CG	1.37	1.49
71:Bf:88:UNK:HG2	71:Bf:91:UNK:CG	1.44	1.43
32:Ao:558:UNK:CG	32:Ao:576:UNK:HG1	1.57	1.34
23:Ae:200:UNK:O	23:Ae:204:UNK:HG3	1.28	1.32
19:Aa:324:UNK:O	19:Aa:328:UNK:HG3	1.32	1.30

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	218/220 (99%)	212 (97%)	6 (3%)	0	100	100
3	AC	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
4	AE	324/328 (99%)	305 (94%)	18 (6%)	1 (0%)	36	67
5	AF	121/124 (98%)	116 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	AG	206/208 (99%)	203 (98%)	3 (2%)	0	100	100
7	AI	291/311 (94%)	283 (97%)	8 (3%)	0	100	100
8	AJ	127/201 (63%)	119 (94%)	6 (5%)	2 (2%)	7	35
9	AK	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
10	AL	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
11	AN	99/128 (77%)	98 (99%)	1 (1%)	0	100	100
12	AO	173/239 (72%)	166 (96%)	7 (4%)	0	100	100
13	AP	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
14	AQ	107/109 (98%)	102 (95%)	5 (5%)	0	100	100
15	AR	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
16	AU	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
19	Aa	243/356 (68%)	238 (98%)	4 (2%)	1 (0%)	30	62
20	Ab	133/190 (70%)	127 (96%)	6 (4%)	0	100	100
21	Ac	167/169 (99%)	157 (94%)	9 (5%)	1 (1%)	21	54
22	Ad	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
24	Af	97/188 (52%)	90 (93%)	7 (7%)	0	100	100
25	Ag	327/397 (82%)	317 (97%)	10 (3%)	0	100	100
26	Ah	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
27	Ai	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
28	Aj	204/218 (94%)	194 (95%)	10 (5%)	0	100	100
29	Ak	273/275 (99%)	265 (97%)	7 (3%)	1 (0%)	30	62
30	Am	114/116 (98%)	108 (95%)	6 (5%)	0	100	100
31	An	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
32	Ao	87/530 (16%)	83 (95%)	4 (5%)	0	100	100
33	Ap	186/188 (99%)	175 (94%)	11 (6%)	0	100	100
36	B0	112/148 (76%)	109 (97%)	3 (3%)	0	100	100
37	B1	242/256 (94%)	237 (98%)	5 (2%)	0	100	100
38	B2	176/252 (70%)	167 (95%)	9 (5%)	0	100	100
39	B3	116/161 (72%)	112 (97%)	4 (3%)	0	100	100
40	B4	43/126 (34%)	40 (93%)	3 (7%)	0	100	100
41	B5	108/188 (57%)	107 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	B6	46/65 (71%)	45 (98%)	1 (2%)	0	100	100
43	B7	44/95 (46%)	44 (100%)	0	0	100	100
44	B8	93/188 (50%)	90 (97%)	3 (3%)	0	100	100
45	B9	36/100 (36%)	36 (100%)	0	0	100	100
48	BD	238/306 (78%)	228 (96%)	10 (4%)	0	100	100
49	BE	305/348 (88%)	278 (91%)	24 (8%)	3 (1%)	12	43
50	BF	248/294 (84%)	232 (94%)	16 (6%)	0	100	100
51	BI	96/268 (36%)	91 (95%)	5 (5%)	0	100	100
52	BJ	166/262 (63%)	158 (95%)	8 (5%)	0	100	100
53	BK	140/192 (73%)	134 (96%)	6 (4%)	0	100	100
54	BN	175/178 (98%)	170 (97%)	5 (3%)	0	100	100
55	BO	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
56	BP	286/296 (97%)	273 (96%)	13 (4%)	0	100	100
57	BQ	219/251 (87%)	218 (100%)	1 (0%)	0	100	100
58	BR	151/169 (89%)	145 (96%)	6 (4%)	0	100	100
59	BS	141/180 (78%)	128 (91%)	12 (8%)	1 (1%)	18	51
60	BT	223/292 (76%)	216 (97%)	7 (3%)	0	100	100
61	BU	138/149 (93%)	132 (96%)	6 (4%)	0	100	100
62	BV	153/209 (73%)	146 (95%)	7 (5%)	0	100	100
63	BW	164/210 (78%)	159 (97%)	5 (3%)	0	100	100
64	BX	130/150 (87%)	126 (97%)	4 (3%)	0	100	100
65	BY	202/216 (94%)	190 (94%)	12 (6%)	0	100	100
66	Ba	391/423 (92%)	374 (96%)	17 (4%)	0	100	100
67	Bb	352/380 (93%)	330 (94%)	21 (6%)	1 (0%)	36	67
68	Bc	293/334 (88%)	281 (96%)	12 (4%)	0	100	100
69	Bd	97/206 (47%)	92 (95%)	5 (5%)	0	100	100
70	Be	119/135 (88%)	115 (97%)	4 (3%)	0	100	100
71	Bf	82/142 (58%)	81 (99%)	1 (1%)	0	100	100
72	Bg	146/159 (92%)	138 (94%)	8 (6%)	0	100	100
73	Bh	287/332 (86%)	269 (94%)	18 (6%)	0	100	100
74	Bi	240/312 (77%)	227 (95%)	12 (5%)	1 (0%)	30	62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	Bj	211/279 (76%)	198 (94%)	12 (6%)	1 (0%)	24	57
76	Bk	132/212 (62%)	125 (95%)	7 (5%)	0	100	100
77	Bl	131/166 (79%)	130 (99%)	1 (1%)	0	100	100
78	Bm	107/159 (67%)	102 (95%)	5 (5%)	0	100	100
79	Bn	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
80	Bo	92/124 (74%)	88 (96%)	4 (4%)	0	100	100
81	Bp	95/112 (85%)	90 (95%)	5 (5%)	0	100	100
82	Bq	35/138 (25%)	34 (97%)	1 (3%)	0	100	100
83	Bt	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
84	Bu	137/205 (67%)	129 (94%)	8 (6%)	0	100	100
85	Bv	118/222 (53%)	116 (98%)	2 (2%)	0	100	100
86	Bw	385/433 (89%)	359 (93%)	25 (6%)	1 (0%)	36	67
87	Bx	160/196 (82%)	154 (96%)	5 (3%)	1 (1%)	21	54
All	All	12706/16216 (78%)	12149 (96%)	542 (4%)	15 (0%)	49	79

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
49	BE	264	ILE
86	Bw	159	VAL
87	Bx	93	ILE
8	AJ	179	GLN
8	AJ	185	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	187/187 (100%)	165 (88%)	22 (12%)	5	22
3	AC	115/115 (100%)	96 (84%)	19 (16%)	2	14
4	AE	273/273 (100%)	237 (87%)	36 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AF	108/109 (99%)	95 (88%)	13 (12%)	5	21
6	AG	181/181 (100%)	165 (91%)	16 (9%)	9	33
7	AI	250/250 (100%)	233 (93%)	17 (7%)	14	40
8	AJ	119/181 (66%)	106 (89%)	13 (11%)	6	25
9	AK	102/102 (100%)	86 (84%)	16 (16%)	2	15
10	AL	92/92 (100%)	80 (87%)	12 (13%)	4	20
11	AN	92/114 (81%)	79 (86%)	13 (14%)	3	18
12	AO	159/205 (78%)	147 (92%)	12 (8%)	12	38
13	AP	97/97 (100%)	91 (94%)	6 (6%)	16	42
14	AQ	94/94 (100%)	84 (89%)	10 (11%)	6	26
15	AR	89/89 (100%)	82 (92%)	7 (8%)	11	36
16	AU	77/77 (100%)	67 (87%)	10 (13%)	4	20
19	Aa	222/272 (82%)	207 (93%)	15 (7%)	14	40
20	Ab	113/162 (70%)	105 (93%)	8 (7%)	13	39
21	Ac	152/152 (100%)	138 (91%)	14 (9%)	8	31
22	Ad	149/149 (100%)	141 (95%)	8 (5%)	20	45
24	Af	86/160 (54%)	79 (92%)	7 (8%)	11	35
25	Ag	290/334 (87%)	263 (91%)	27 (9%)	8	30
26	Ah	95/95 (100%)	93 (98%)	2 (2%)	47	64
27	Ai	86/86 (100%)	77 (90%)	9 (10%)	6	26
28	Aj	182/184 (99%)	172 (94%)	10 (6%)	19	45
29	Ak	249/249 (100%)	224 (90%)	25 (10%)	7	28
30	Am	100/100 (100%)	91 (91%)	9 (9%)	9	32
31	An	66/66 (100%)	57 (86%)	9 (14%)	3	18
32	Ao	79/118 (67%)	73 (92%)	6 (8%)	12	37
33	Ap	168/168 (100%)	152 (90%)	16 (10%)	8	30
36	B0	92/115 (80%)	76 (83%)	16 (17%)	2	12
37	B1	219/229 (96%)	194 (89%)	25 (11%)	5	23
38	B2	164/228 (72%)	143 (87%)	21 (13%)	4	21
39	B3	110/147 (75%)	96 (87%)	14 (13%)	4	21
40	B4	42/114 (37%)	39 (93%)	3 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	B5	99/163 (61%)	91 (92%)	8 (8%)	11	35
42	B6	45/60 (75%)	36 (80%)	9 (20%)	1	8
43	B7	41/78 (53%)	35 (85%)	6 (15%)	3	17
44	B8	87/162 (54%)	76 (87%)	11 (13%)	4	21
45	B9	36/77 (47%)	32 (89%)	4 (11%)	6	24
48	BD	193/248 (78%)	157 (81%)	36 (19%)	1	10
49	BE	263/290 (91%)	238 (90%)	25 (10%)	8	30
50	BF	217/251 (86%)	185 (85%)	32 (15%)	3	17
51	BI	88/228 (39%)	83 (94%)	5 (6%)	18	44
52	BJ	154/230 (67%)	140 (91%)	14 (9%)	9	32
53	BK	115/151 (76%)	109 (95%)	6 (5%)	21	46
54	BN	156/157 (99%)	134 (86%)	22 (14%)	3	18
55	BO	99/123 (80%)	87 (88%)	12 (12%)	5	21
56	BP	245/249 (98%)	204 (83%)	41 (17%)	2	13
57	BQ	189/210 (90%)	167 (88%)	22 (12%)	5	22
58	BR	132/143 (92%)	112 (85%)	20 (15%)	3	16
59	BS	123/153 (80%)	109 (89%)	14 (11%)	5	23
60	BT	206/243 (85%)	178 (86%)	28 (14%)	3	18
61	BU	118/127 (93%)	102 (86%)	16 (14%)	3	18
62	BV	136/178 (76%)	113 (83%)	23 (17%)	2	13
63	BW	144/180 (80%)	121 (84%)	23 (16%)	2	14
64	BX	119/134 (89%)	99 (83%)	20 (17%)	2	13
65	BY	183/192 (95%)	157 (86%)	26 (14%)	3	17
66	Ba	348/365 (95%)	302 (87%)	46 (13%)	4	19
67	Bb	310/328 (94%)	277 (89%)	33 (11%)	6	26
68	Bc	271/299 (91%)	248 (92%)	23 (8%)	10	33
69	Bd	92/181 (51%)	84 (91%)	8 (9%)	9	33
70	Be	100/108 (93%)	87 (87%)	13 (13%)	4	20
71	Bf	80/110 (73%)	67 (84%)	13 (16%)	2	14
72	Bg	128/136 (94%)	108 (84%)	20 (16%)	2	15
73	Bh	251/284 (88%)	223 (89%)	28 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
74	Bi	218/281 (78%)	198 (91%)	20 (9%)	8	31
75	Bj	190/242 (78%)	174 (92%)	16 (8%)	10	34
76	Bk	119/181 (66%)	109 (92%)	10 (8%)	10	34
77	Bl	122/147 (83%)	100 (82%)	22 (18%)	2	12
78	Bm	103/145 (71%)	96 (93%)	7 (7%)	14	40
79	Bn	88/113 (78%)	74 (84%)	14 (16%)	2	14
80	Bo	74/97 (76%)	62 (84%)	12 (16%)	2	14
81	Bp	79/88 (90%)	73 (92%)	6 (8%)	12	37
82	Bq	36/114 (32%)	35 (97%)	1 (3%)	38	58
83	Bt	75/82 (92%)	60 (80%)	15 (20%)	1	8
84	Bu	126/169 (75%)	118 (94%)	8 (6%)	16	42
85	Bv	102/173 (59%)	97 (95%)	5 (5%)	22	47
86	Bw	340/373 (91%)	290 (85%)	50 (15%)	3	17
87	Bx	149/173 (86%)	130 (87%)	19 (13%)	4	21
All	All	11288/13510 (84%)	10010 (89%)	1278 (11%)	8	23

5 of 1278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
66	Ba	370	VAL
78	Bm	142	ASP
67	Bb	279	ILE
66	Ba	355	LEU
72	Bg	119	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 302 such sidechains are listed below:

Mol	Chain	Res	Type
68	Bc	310	ASN
84	Bu	183	ASN
71	Bf	121	HIS
76	Bk	92	ASN
87	Bx	170	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	959/962 (99%)	308 (32%)	7 (0%)
17	AV	66/69 (95%)	12 (18%)	0
17	AY	65/69 (94%)	16 (24%)	0
18	AX	12/13 (92%)	4 (33%)	0
46	BA	1508/1570 (96%)	622 (41%)	30 (1%)
47	BB	48/51 (94%)	13 (27%)	0
All	All	2658/2734 (97%)	975 (36%)	37 (1%)

5 of 975 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	A
1	AA	10	U
1	AA	11	G
1	AA	14	C
1	AA	18	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
46	BA	583	A
46	BA	1431	U
46	BA	653	C
46	BA	936	U
46	BA	112	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

202 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	AX	12	-	14,16,20	4.30	2 (14%)	19,22,29	1.01	1 (5%)
17	Y5P	AV	1	-	14,16,20	4.63	3 (21%)	19,22,29	1.13	2 (10%)
17	Y5P	AY	1	-	14,16,20	4.65	3 (21%)	19,22,29	1.06	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	Y5P	BB	6	47	14,19,20	4.24	2 (14%)	18,26,29	0.99	1 (5%)
47	Y5P	BB	40	47	14,19,20	4.22	2 (14%)	18,26,29	1.01	1 (5%)
17	Y5P	AV	12	-	14,19,20	4.30	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	67	-	14,19,20	4.63	2 (14%)	18,26,29	1.34	2 (11%)
47	P5P	BB	37	47	20,23,24	0.46	0	27,33,36	0.89	1 (3%)
17	Y5P	AV	52	-	14,19,20	4.66	3 (21%)	18,26,29	1.12	1 (5%)
17	Y5P	AY	37	-	14,19,20	4.67	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AY	29	-	14,19,20	4.65	3 (21%)	18,26,29	1.08	1 (5%)
17	Y5P	AV	13	-	14,19,20	4.55	2 (14%)	18,26,29	1.36	2 (11%)
17	Y5P	AY	30	-	14,19,20	4.65	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	66	-	14,19,20	4.40	2 (14%)	18,26,29	1.02	1 (5%)
18	Y5P	AX	17	-	14,19,20	4.17	2 (14%)	18,26,29	0.98	1 (5%)
17	Y5P	AV	49	-	14,19,20	4.62	2 (14%)	18,26,29	1.33	2 (11%)
17	Y5P	AV	24	-	14,19,20	4.66	3 (21%)	18,26,29	1.06	1 (5%)
17	Y5P	AY	33	-	14,19,20	4.25	2 (14%)	18,26,29	1.03	1 (5%)
47	P5P	BB	9	47	20,23,24	0.43	0	27,33,36	0.78	1 (3%)
17	Y5P	AV	45	-	14,19,20	4.44	2 (14%)	18,26,29	0.97	1 (5%)
18	Y5P	AX	22	-	14,19,20	4.36	2 (14%)	18,26,29	1.12	1 (5%)
17	Y5P	AV	29	-	14,19,20	4.60	3 (21%)	18,26,29	1.18	1 (5%)
17	Y5P	AY	73	-	14,19,20	4.73	3 (21%)	18,26,29	1.47	3 (16%)
47	Y5P	BB	11	47	14,19,20	4.68	2 (14%)	18,26,29	1.29	1 (5%)
17	Y5P	AV	65	-	14,19,20	4.66	3 (21%)	18,26,29	1.06	1 (5%)
17	Y5P	AY	51	-	14,19,20	4.30	2 (14%)	18,26,29	1.05	1 (5%)
17	Y5P	AV	33	-	14,19,20	4.32	2 (14%)	18,26,29	0.93	1 (5%)
17	Y5P	AY	65	-	14,19,20	4.67	3 (21%)	18,26,29	1.08	1 (5%)
17	Y5P	AV	68	-	14,19,20	4.61	2 (14%)	18,26,29	1.32	2 (11%)
17	Y5P	AV	2	-	14,19,20	4.72	2 (14%)	18,26,29	1.17	1 (5%)
17	Y5P	AV	69	-	14,19,20	4.68	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AV	73	-	14,19,20	4.71	3 (21%)	18,26,29	1.32	3 (16%)
17	Y5P	AY	44	-	14,19,20	4.69	3 (21%)	18,26,29	1.06	1 (5%)
18	Y5P	AX	16	-	14,19,20	4.16	2 (14%)	18,26,29	1.08	1 (5%)
17	Y5P	AV	31	-	14,19,20	4.66	3 (21%)	18,26,29	1.05	1 (5%)
47	P5P	BB	29	47	20,23,24	1.01	2 (10%)	27,33,36	1.91	3 (11%)
17	Y5P	AV	21	-	14,19,20	4.71	3 (21%)	18,26,29	1.15	1 (5%)
17	Y5P	AY	2	-	14,19,20	4.65	2 (14%)	18,26,29	1.27	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	Y5P	AY	13	-	14,19,20	4.57	2 (14%)	18,26,29	1.37	2 (11%)
17	Y5P	AY	66	-	14,19,20	4.27	2 (14%)	18,26,29	1.05	1 (5%)
17	Y5P	AY	27	-	14,19,20	4.65	3 (21%)	18,26,29	1.21	2 (11%)
17	Y5P	AV	44	-	14,19,20	4.69	3 (21%)	18,26,29	1.09	1 (5%)
47	Y5P	BB	63	47	14,19,20	4.67	2 (14%)	18,26,29	1.28	2 (11%)
47	P5P	BB	36	47	20,23,24	0.48	0	27,33,36	0.80	1 (3%)
17	Y5P	AV	5	-	14,19,20	4.66	3 (21%)	18,26,29	1.05	1 (5%)
17	Y5P	AV	4	-	14,19,20	4.60	2 (14%)	18,26,29	1.29	2 (11%)
17	Y5P	AY	6	-	14,19,20	4.65	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	54	-	14,19,20	4.37	2 (14%)	18,26,29	1.02	1 (5%)
17	Y5P	AV	61	-	14,19,20	4.58	2 (14%)	18,26,29	1.33	2 (11%)
17	Y5P	AY	32	-	14,19,20	4.22	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AY	15	-	14,19,20	4.66	3 (21%)	18,26,29	1.14	2 (11%)
17	Y5P	AY	61	-	14,19,20	4.51	2 (14%)	18,26,29	1.42	2 (11%)
47	Y5P	BB	43	47	14,19,20	4.55	2 (14%)	18,26,29	1.43	2 (11%)
17	Y5P	AY	62	-	14,19,20	4.58	2 (14%)	18,26,29	1.40	2 (11%)
17	Y5P	AY	41	-	14,19,20	4.56	2 (14%)	18,26,29	1.42	2 (11%)
47	P5P	BB	25	47	20,23,24	1.04	3 (15%)	27,33,36	1.91	4 (14%)
17	Y5P	AV	27	-	14,19,20	4.71	3 (21%)	18,26,29	1.14	2 (11%)
17	Y5P	AY	43	-	14,19,20	4.55	2 (14%)	18,26,29	1.36	2 (11%)
17	Y5P	AV	23	-	14,19,20	4.65	3 (21%)	18,26,29	1.05	1 (5%)
47	Y5P	BB	34	47	14,19,20	4.42	2 (14%)	18,26,29	1.03	1 (5%)
47	P5P	BB	64	47	20,23,24	0.50	0	27,33,36	0.72	1 (3%)
17	Y5P	AY	60	-	14,19,20	4.27	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AV	9	-	14,19,20	4.65	3 (21%)	18,26,29	1.11	1 (5%)
47	P5P	BB	32	47	20,23,24	0.49	0	27,33,36	0.70	0
17	Y5P	AY	52	-	14,19,20	4.63	3 (21%)	18,26,29	1.13	1 (5%)
17	Y5P	AV	10	-	14,19,20	4.64	3 (21%)	18,26,29	1.11	1 (5%)
17	Y5P	AV	25	-	14,19,20	4.71	2 (14%)	18,26,29	1.27	1 (5%)
47	P5P	BB	5	47	20,23,24	0.48	0	27,33,36	0.71	1 (3%)
47	P5P	BB	49	47	20,23,24	1.05	3 (15%)	27,33,36	1.90	4 (14%)
47	P5P	BB	10	47	20,23,24	0.90	2 (10%)	27,33,36	1.91	3 (11%)
17	Y5P	AV	39	-	14,19,20	4.22	2 (14%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	30	-	14,19,20	4.68	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AY	39	-	14,19,20	4.21	2 (14%)	18,26,29	1.04	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	P5P	BB	7	47	20,23,24	0.97	3 (15%)	27,33,36	1.97	3 (11%)
17	Y5P	AY	53	-	14,19,20	4.65	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AY	4	-	14,19,20	4.66	2 (14%)	18,26,29	1.36	2 (11%)
17	Y5P	AY	12	-	14,19,20	4.24	2 (14%)	18,26,29	1.01	1 (5%)
47	Y5P	BB	53	47	14,19,20	4.59	2 (14%)	18,26,29	1.37	2 (11%)
17	Y5P	AY	70	-	14,19,20	4.68	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AY	10	-	14,19,20	4.64	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AV	53	-	14,19,20	4.65	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	14	-	14,19,20	4.65	3 (21%)	18,26,29	1.02	1 (5%)
17	Y5P	AY	28	-	14,19,20	4.66	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	26	-	14,19,20	4.66	3 (21%)	18,26,29	1.08	1 (5%)
17	Y5P	AY	63	-	14,19,20	4.63	3 (21%)	18,26,29	1.06	1 (5%)
47	P5P	BB	39	47	20,23,24	0.53	0	27,33,36	0.74	1 (3%)
47	P5P	BB	30	47	20,23,24	1.03	2 (10%)	27,33,36	1.74	4 (14%)
17	P5P	AV	35	-	20,23,24	0.47	0	27,33,36	0.78	1 (3%)
17	Y5P	AY	59	-	14,19,20	4.31	2 (14%)	18,26,29	1.00	1 (5%)
17	P5P	AY	35	-	20,23,24	0.48	0	27,33,36	0.77	1 (3%)
47	Y5P	BB	8	47	14,19,20	4.27	2 (14%)	18,26,29	1.08	1 (5%)
47	Y5P	BB	60	47	14,19,20	4.50	2 (14%)	18,26,29	1.40	2 (11%)
47	P5P	BB	15	47	20,23,24	0.49	0	27,33,36	0.69	1 (3%)
47	Y5P	BB	61	47	14,19,20	4.28	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AY	45	-	14,19,20	4.20	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	14	-	14,19,20	4.67	3 (21%)	18,26,29	1.11	1 (5%)
17	Y5P	AY	50	-	14,19,20	4.25	2 (14%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	74	-	14,19,20	4.67	2 (14%)	18,26,29	1.26	2 (11%)
17	Y5P	AY	38	-	14,19,20	4.64	3 (21%)	18,26,29	1.06	1 (5%)
18	Y5P	AX	20	-	14,19,20	4.21	2 (14%)	18,26,29	1.05	1 (5%)
47	P5P	BB	51	47	20,23,24	0.98	2 (10%)	27,33,36	1.91	4 (14%)
17	Y5P	AY	9	-	14,19,20	4.64	3 (21%)	18,26,29	1.06	1 (5%)
47	P5P	BB	45	47	20,23,24	0.47	0	27,33,36	0.71	0
17	Y5P	AV	38	-	14,19,20	4.64	3 (21%)	18,26,29	1.05	1 (5%)
17	Y5P	AY	22	-	14,19,20	4.65	3 (21%)	18,26,29	1.08	1 (5%)
17	Y5P	AY	40	-	14,19,20	4.48	2 (14%)	18,26,29	1.43	2 (11%)
47	Y5P	BB	33	47	14,19,20	4.56	2 (14%)	18,26,29	1.37	2 (11%)
17	Y5P	AY	49	-	14,19,20	4.49	2 (14%)	18,26,29	1.40	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	Y5P	AV	50	-	14,19,20	4.40	2 (14%)	18,26,29	0.99	1 (5%)
18	Y5P	AX	21	-	14,19,20	4.57	2 (14%)	18,26,29	1.41	2 (11%)
17	Y5P	AV	22	-	14,19,20	4.67	3 (21%)	18,26,29	1.09	1 (5%)
17	Y5P	AV	72	-	14,19,20	4.67	2 (14%)	18,26,29	1.33	1 (5%)
17	Y5P	AY	72	-	14,19,20	4.70	2 (14%)	18,26,29	1.26	1 (5%)
47	Y5P	BB	31	47	14,19,20	4.63	2 (14%)	18,26,29	1.35	2 (11%)
17	Y5P	AV	6	-	14,19,20	4.65	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	43	-	14,19,20	4.72	2 (14%)	18,26,29	1.24	2 (11%)
47	P5P	BB	38	47	20,23,24	0.54	0	27,33,36	0.77	1 (3%)
18	Y5P	AX	14	-	14,19,20	4.42	2 (14%)	18,26,29	0.97	1 (5%)
47	P5P	BB	27	47	20,23,24	0.48	0	27,33,36	0.85	0
17	Y5P	AV	51	-	14,19,20	4.38	2 (14%)	18,26,29	1.00	1 (5%)
17	P5P	AV	36	-	20,23,24	0.48	0	27,33,36	0.74	1 (3%)
47	P5P	BB	46	47	20,23,24	0.93	3 (15%)	27,33,36	1.83	3 (11%)
17	Y5P	AY	11	-	14,19,20	4.58	2 (14%)	18,26,29	1.35	2 (11%)
17	Y5P	AY	71	-	14,19,20	4.67	3 (21%)	18,26,29	1.14	1 (5%)
17	Y5P	AY	5	-	14,19,20	4.65	3 (21%)	18,26,29	1.10	1 (5%)
47	Y5P	BB	62	47	14,19,20	4.33	2 (14%)	18,26,29	1.01	1 (5%)
18	Y5P	AX	23	-	14,19,20	4.33	2 (14%)	18,26,29	1.02	1 (5%)
47	P5P	BB	35	47	20,23,24	1.11	3 (15%)	27,33,36	1.87	3 (11%)
47	Y5P	BB	44	47	14,19,20	4.26	2 (14%)	18,26,29	0.96	1 (5%)
17	Y5P	AV	11	-	14,19,20	4.50	2 (14%)	18,26,29	1.44	2 (11%)
47	P5P	BB	14	47	20,23,24	0.48	0	27,33,36	0.79	1 (3%)
17	Y5P	AV	48	-	14,19,20	4.56	2 (14%)	18,26,29	1.49	2 (11%)
17	Y5P	AY	7	-	14,19,20	4.65	3 (21%)	18,26,29	1.05	1 (5%)
17	Y5P	AY	55	-	14,19,20	4.42	2 (14%)	18,26,29	1.14	2 (11%)
47	Y5P	BB	12	47	14,19,20	4.31	2 (14%)	18,26,29	0.99	1 (5%)
17	Y5P	AV	71	-	14,19,20	4.65	3 (21%)	18,26,29	1.05	1 (5%)
17	P5P	AY	34	-	20,23,24	1.00	2 (10%)	27,33,36	2.00	3 (11%)
17	P5P	AY	36	-	20,23,24	0.54	0	27,33,36	0.80	1 (3%)
17	Y5P	AV	8	-	14,19,20	4.12	2 (14%)	18,26,29	1.13	1 (5%)
17	Y5P	AY	25	-	14,19,20	4.54	2 (14%)	18,26,29	1.34	2 (11%)
47	P5P	BB	41	47	20,23,24	1.00	2 (10%)	27,33,36	1.95	4 (14%)
17	Y5P	AV	7	-	14,19,20	4.61	3 (21%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	8	-	14,19,20	4.23	2 (14%)	18,26,29	1.03	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	Y5P	AV	40	-	14,19,20	4.63	2 (14%)	18,26,29	1.34	2 (11%)
17	Y5P	AV	55	-	14,19,20	4.30	2 (14%)	18,26,29	1.06	1 (5%)
17	Y5P	AY	67	-	14,19,20	4.63	2 (14%)	18,26,29	1.40	1 (5%)
17	Y5P	AY	3	-	14,19,20	4.50	2 (14%)	18,26,29	1.43	2 (11%)
47	P5P	BB	58	47	20,23,24	0.49	0	27,33,36	0.70	1 (3%)
17	Y5P	AV	59	-	14,19,20	4.32	2 (14%)	18,26,29	1.00	1 (5%)
18	Y5P	AX	15	-	14,19,20	4.43	2 (14%)	18,26,29	1.06	1 (5%)
17	Y5P	AV	58	-	14,19,20	4.67	3 (21%)	18,26,29	1.12	1 (5%)
18	Y5P	AX	24	-	14,19,20	4.51	2 (14%)	18,26,29	0.94	1 (5%)
17	Y5P	AV	74	-	14,19,20	4.70	2 (14%)	18,26,29	1.21	2 (11%)
17	Y5P	AY	48	-	14,19,20	4.53	2 (14%)	18,26,29	1.36	2 (11%)
47	Y5P	BB	42	47	14,19,20	4.54	2 (14%)	18,26,29	1.44	2 (11%)
17	Y5P	AY	31	-	14,19,20	4.65	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	75	-	14,19,20	4.59	2 (14%)	18,26,29	1.34	2 (11%)
47	Y5P	BB	48	47	14,19,20	4.28	2 (14%)	18,26,29	1.03	1 (5%)
17	Y5P	AY	21	-	14,19,20	4.65	3 (21%)	18,26,29	1.07	1 (5%)
47	P5P	BB	24	47	20,23,24	0.46	0	27,33,36	0.84	0
47	Y5P	BB	13	47	14,19,20	4.20	2 (14%)	18,26,29	1.23	1 (5%)
17	Y5P	AV	63	-	14,19,20	4.67	3 (21%)	18,26,29	1.06	1 (5%)
17	Y5P	AV	62	-	14,19,20	4.52	2 (14%)	18,26,29	1.38	2 (11%)
17	Y5P	AV	41	-	14,19,20	4.63	2 (14%)	18,26,29	1.37	2 (11%)
47	Y5P	BB	26	47	14,19,20	4.55	2 (14%)	18,26,29	1.40	2 (11%)
17	Y5P	AY	24	-	14,19,20	4.64	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AV	37	-	14,19,20	4.67	3 (21%)	18,26,29	1.07	1 (5%)
18	Y5P	AX	19	-	14,19,20	4.28	2 (14%)	18,26,29	0.95	1 (5%)
17	Y5P	AY	68	-	14,19,20	4.58	2 (14%)	18,26,29	1.30	2 (11%)
17	Y5P	AV	56	-	14,19,20	4.61	2 (14%)	18,26,29	1.30	2 (11%)
47	Y5P	BB	52	47	14,19,20	4.61	2 (14%)	18,26,29	1.34	2 (11%)
17	Y5P	AY	56	-	14,19,20	4.58	2 (14%)	18,26,29	1.33	2 (11%)
47	P5P	BB	47	47	20,23,24	0.40	0	27,33,36	0.90	2 (7%)
17	Y5P	AV	75	-	14,19,20	4.37	2 (14%)	18,26,29	1.43	2 (11%)
17	Y5P	AV	60	-	14,19,20	4.34	2 (14%)	18,26,29	1.08	1 (5%)
17	P5P	AY	76	46	20,23,24	0.60	1 (5%)	27,33,36	0.74	1 (3%)
17	Y5P	AY	23	-	14,19,20	4.67	3 (21%)	18,26,29	1.03	1 (5%)
47	P5P	BB	59	47	20,23,24	1.01	3 (15%)	27,33,36	1.86	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	Y5P	AX	18	-	14,19,20	4.54	2 (14%)	18,26,29	1.30	2 (11%)
17	Y5P	AY	58	-	14,19,20	4.64	3 (21%)	18,26,29	1.12	1 (5%)
17	Y5P	AY	69	-	14,19,20	4.67	3 (21%)	18,26,29	1.22	2 (11%)
17	Y5P	AY	57	-	14,19,20	4.67	3 (21%)	18,26,29	1.03	1 (5%)
17	P5P	AV	76	46	20,23,24	0.54	0	27,33,36	0.81	1 (3%)
17	P5P	AV	34	-	20,23,24	1.13	3 (15%)	27,33,36	2.00	4 (14%)
17	Y5P	AV	57	-	14,19,20	4.73	3 (21%)	18,26,29	1.12	1 (5%)
17	Y5P	AY	64	-	14,19,20	4.68	3 (21%)	18,26,29	1.11	1 (5%)
47	Y5P	BB	65	47	14,19,20	4.19	2 (14%)	18,26,29	1.09	1 (5%)
47	P5P	BB	28	47	20,23,24	0.49	0	27,33,36	0.72	1 (3%)
17	Y5P	AY	26	-	14,19,20	4.70	3 (21%)	18,26,29	1.05	1 (5%)
47	P5P	BB	23	47	20,23,24	0.55	0	27,33,36	1.33	4 (14%)
17	Y5P	AY	42	-	14,19,20	4.58	2 (14%)	18,26,29	1.47	2 (11%)
17	Y5P	AV	3	-	14,19,20	4.70	2 (14%)	18,26,29	1.28	2 (11%)
18	Y5P	AX	13	-	14,19,20	4.34	2 (14%)	18,26,29	1.02	1 (5%)
17	Y5P	AV	64	-	14,19,20	4.69	3 (21%)	18,26,29	1.04	1 (5%)
17	Y5P	AY	54	-	14,19,20	4.25	2 (14%)	18,26,29	1.05	1 (5%)
47	P5P	BB	50	47	20,23,24	0.51	0	27,33,36	0.77	0
17	Y5P	AV	32	-	14,19,20	4.34	2 (14%)	18,26,29	1.00	1 (5%)
17	Y5P	AV	15	-	14,19,20	4.63	3 (21%)	18,26,29	1.03	1 (5%)
17	Y5P	AV	42	-	14,19,20	4.63	2 (14%)	18,26,29	1.27	2 (11%)
17	Y5P	AV	70	-	14,19,20	4.67	3 (21%)	18,26,29	1.07	1 (5%)
17	Y5P	AV	28	-	14,19,20	4.63	3 (21%)	18,26,29	1.03	1 (5%)
47	P5P	BB	66	47	20,23,24	0.45	0	27,33,36	0.74	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	Y5P	AX	12	-	-	3/6/30/34	0/2/2/2
17	Y5P	AV	1	-	-	1/6/30/34	0/2/2/2
17	Y5P	AY	1	-	-	1/6/30/34	0/2/2/2
47	Y5P	BB	6	47	-	1/7/33/34	0/2/2/2
47	Y5P	BB	40	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	12	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	67	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	37	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	52	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	37	-	-	4/7/33/34	0/2/2/2
17	Y5P	AY	29	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	13	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	30	-	-	4/7/33/34	0/2/2/2
17	Y5P	AV	66	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	17	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	49	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	24	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	33	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	9	47	-	4/7/25/26	0/3/3/3
17	Y5P	AV	45	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	22	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	29	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	73	-	-	2/7/33/34	0/2/2/2
47	Y5P	BB	11	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	65	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	51	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	33	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	65	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	68	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	2	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	69	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	73	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	44	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	16	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	31	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	29	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	21	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	2	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	13	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	66	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	27	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	44	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	63	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	36	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	5	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	4	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	6	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	54	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	61	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	32	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	15	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	61	-	-	3/7/33/34	0/2/2/2
47	Y5P	BB	43	47	-	3/7/33/34	0/2/2/2
17	Y5P	AY	62	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	41	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	25	47	-	2/7/25/26	0/3/3/3
17	Y5P	AV	27	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	43	-	-	4/7/33/34	0/2/2/2
17	Y5P	AV	23	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	34	47	-	3/7/33/34	0/2/2/2
47	P5P	BB	64	47	-	0/7/25/26	0/3/3/3
17	Y5P	AY	60	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	9	-	-	5/7/33/34	0/2/2/2
47	P5P	BB	32	47	-	0/7/25/26	0/3/3/3
17	Y5P	AY	52	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	10	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	25	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	5	47	-	3/7/25/26	0/3/3/3
47	P5P	BB	49	47	-	2/7/25/26	0/3/3/3
47	P5P	BB	10	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	39	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	30	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	39	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	7	47	-	1/7/25/26	0/3/3/3
17	Y5P	AY	53	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	4	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	12	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	53	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	70	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	10	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	53	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	14	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	28	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	26	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	63	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	39	47	-	0/7/25/26	0/3/3/3
47	P5P	BB	30	47	-	0/7/25/26	0/3/3/3
17	P5P	AV	35	-	-	0/7/25/26	0/3/3/3
17	Y5P	AY	59	-	-	2/7/33/34	0/2/2/2
17	P5P	AY	35	-	-	0/7/25/26	0/3/3/3
47	Y5P	BB	8	47	-	2/7/33/34	0/2/2/2
47	Y5P	BB	60	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	15	47	-	2/7/25/26	0/3/3/3
47	Y5P	BB	61	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	45	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	14	-	-	5/7/33/34	0/2/2/2
17	Y5P	AY	50	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	74	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	38	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	20	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	51	47	-	0/7/25/26	0/3/3/3
17	Y5P	AY	9	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	45	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	38	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	22	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	40	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	33	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	49	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	50	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	21	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	22	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	72	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	72	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	31	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	6	-	-	4/7/33/34	0/2/2/2
17	Y5P	AV	43	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	38	47	-	0/7/25/26	0/3/3/3
18	Y5P	AX	14	-	-	2/7/33/34	0/2/2/2
47	P5P	BB	27	47	-	1/7/25/26	0/3/3/3
17	Y5P	AV	51	-	-	1/7/33/34	0/2/2/2
17	P5P	AV	36	-	-	0/7/25/26	0/3/3/3
47	P5P	BB	46	47	-	3/7/25/26	0/3/3/3
17	Y5P	AY	11	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	71	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AY	5	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	62	47	-	1/7/33/34	0/2/2/2
18	Y5P	AX	23	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	35	47	-	2/7/25/26	0/3/3/3
47	Y5P	BB	44	47	-	3/7/33/34	0/2/2/2
17	Y5P	AV	11	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	14	47	-	2/7/25/26	0/3/3/3
17	Y5P	AV	48	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	7	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	55	-	-	2/7/33/34	0/2/2/2
47	Y5P	BB	12	47	-	3/7/33/34	0/2/2/2
17	Y5P	AV	71	-	-	1/7/33/34	0/2/2/2
17	P5P	AY	34	-	-	2/7/25/26	0/3/3/3
17	P5P	AY	36	-	-	0/7/25/26	0/3/3/3
17	Y5P	AV	8	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	25	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	41	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	7	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	8	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	40	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	55	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	67	-	-	3/7/33/34	0/2/2/2
17	Y5P	AY	3	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	58	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	59	-	-	3/7/33/34	0/2/2/2
18	Y5P	AX	15	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	58	-	-	4/7/33/34	0/2/2/2
18	Y5P	AX	24	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	74	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	48	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	42	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	31	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	75	-	-	2/7/33/34	0/2/2/2
47	Y5P	BB	48	47	-	3/7/33/34	0/2/2/2
17	Y5P	AY	21	-	-	3/7/33/34	0/2/2/2
47	P5P	BB	24	47	-	2/7/25/26	0/3/3/3
47	Y5P	BB	13	47	-	1/7/33/34	0/2/2/2
17	Y5P	AV	63	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	Y5P	AV	62	-	-	2/7/33/34	0/2/2/2
17	Y5P	AV	41	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	26	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	24	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	37	-	-	2/7/33/34	0/2/2/2
18	Y5P	AX	19	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	68	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	56	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	52	47	-	1/7/33/34	0/2/2/2
17	Y5P	AY	56	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	47	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	75	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	60	-	-	1/7/33/34	0/2/2/2
17	P5P	AY	76	46	-	0/7/25/26	0/3/3/3
17	Y5P	AY	23	-	-	2/7/33/34	0/2/2/2
47	P5P	BB	59	47	-	0/7/25/26	0/3/3/3
18	Y5P	AX	18	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	58	-	-	4/7/33/34	0/2/2/2
17	Y5P	AY	69	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	57	-	-	1/7/33/34	0/2/2/2
17	P5P	AV	76	46	-	1/7/25/26	0/3/3/3
17	P5P	AV	34	-	-	0/7/25/26	0/3/3/3
17	Y5P	AV	57	-	-	2/7/33/34	0/2/2/2
17	Y5P	AY	64	-	-	1/7/33/34	0/2/2/2
47	Y5P	BB	65	47	-	1/7/33/34	0/2/2/2
47	P5P	BB	28	47	-	0/7/25/26	0/3/3/3
17	Y5P	AY	26	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	23	47	-	2/7/25/26	0/3/3/3
17	Y5P	AY	42	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	3	-	-	1/7/33/34	0/2/2/2
18	Y5P	AX	13	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	64	-	-	1/7/33/34	0/2/2/2
17	Y5P	AY	54	-	-	1/7/33/34	0/2/2/2
47	P5P	BB	50	47	-	0/7/25/26	0/3/3/3
17	Y5P	AV	32	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	15	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	42	-	-	3/7/33/34	0/2/2/2
17	Y5P	AV	70	-	-	1/7/33/34	0/2/2/2
17	Y5P	AV	28	-	-	1/7/33/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	P5P	BB	66	47	-	0/7/25/26	0/3/3/3

The worst 5 of 426 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	AX	24	Y5P	C2-N3	14.77	1.38	1.27
18	AX	15	Y5P	C2-N3	14.73	1.38	1.27
17	AV	69	Y5P	C2-N3	14.48	1.38	1.27
17	AV	63	Y5P	C2-N3	14.48	1.38	1.27
17	AV	57	Y5P	C2-N3	14.47	1.38	1.27

The worst 5 of 290 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	AV	34	P5P	C6-N1-C2	8.50	125.83	115.80
47	BB	7	P5P	C6-N1-C2	8.24	125.52	115.80
47	BB	41	P5P	C6-N1-C2	8.16	125.43	115.80
17	AY	34	P5P	C6-N1-C2	8.14	125.41	115.80
47	BB	49	P5P	C6-N1-C2	7.97	125.20	115.80

There are no chirality outliers.

5 of 296 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	AV	76	P5P	C4'-C5'-O5'-P
17	AY	34	P5P	O4'-C4'-C5'-O5'
47	BB	5	P5P	O4'-C4'-C5'-O5'
47	BB	15	P5P	O4'-C4'-C5'-O5'
47	BB	23	P5P	C4'-C5'-O5'-P

There are no ring outliers.

140 monomers are involved in 187 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	AX	12	Y5P	1	0
17	AV	12	Y5P	1	0
17	AV	67	Y5P	4	0
47	BB	37	P5P	2	0
17	AV	52	Y5P	2	0
17	AY	37	Y5P	3	0
17	AY	29	Y5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AV	13	Y5P	1	0
17	AY	30	Y5P	2	0
17	AV	66	Y5P	3	0
18	AX	17	Y5P	1	0
17	AV	49	Y5P	1	0
17	AV	24	Y5P	2	0
17	AY	33	Y5P	2	0
47	BB	9	P5P	2	0
18	AX	22	Y5P	1	0
17	AV	29	Y5P	4	0
47	BB	11	Y5P	1	0
17	AV	65	Y5P	1	0
17	AY	51	Y5P	1	0
17	AV	33	Y5P	1	0
17	AV	68	Y5P	1	0
17	AV	2	Y5P	2	0
17	AY	44	Y5P	1	0
18	AX	16	Y5P	1	0
17	AV	31	Y5P	2	0
47	BB	29	P5P	3	0
17	AV	21	Y5P	1	0
17	AY	2	Y5P	1	0
17	AY	66	Y5P	1	0
17	AY	27	Y5P	1	0
17	AV	44	Y5P	4	0
47	BB	63	Y5P	1	0
47	BB	36	P5P	1	0
17	AV	5	Y5P	1	0
17	AV	4	Y5P	1	0
17	AY	6	Y5P	3	0
17	AV	54	Y5P	6	0
17	AY	32	Y5P	4	0
17	AY	15	Y5P	1	0
17	AY	61	Y5P	1	0
47	BB	43	Y5P	2	0
17	AY	62	Y5P	2	0
47	BB	25	P5P	3	0
17	AV	27	Y5P	4	0
17	AY	43	Y5P	2	0
47	BB	34	Y5P	1	0
17	AV	9	Y5P	2	0
47	BB	32	P5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AY	52	Y5P	1	0
17	AV	10	Y5P	4	0
17	AV	25	Y5P	3	0
17	AV	30	Y5P	3	0
17	AY	39	Y5P	2	0
17	AY	53	Y5P	1	0
17	AY	4	Y5P	1	0
17	AY	12	Y5P	1	0
17	AY	70	Y5P	2	0
17	AV	53	Y5P	2	0
17	AY	14	Y5P	6	0
17	AY	28	Y5P	2	0
17	AV	26	Y5P	2	0
17	AY	63	Y5P	1	0
47	BB	39	P5P	2	0
47	BB	30	P5P	3	0
17	AV	35	P5P	1	0
47	BB	61	Y5P	2	0
17	AY	45	Y5P	1	0
17	AV	14	Y5P	1	0
17	AY	50	Y5P	1	0
17	AY	74	Y5P	2	0
17	AY	38	Y5P	3	0
18	AX	20	Y5P	1	0
17	AY	9	Y5P	6	0
47	BB	45	P5P	1	0
17	AV	38	Y5P	4	0
17	AY	22	Y5P	6	0
47	BB	33	Y5P	2	0
17	AV	50	Y5P	1	0
18	AX	21	Y5P	3	0
47	BB	31	Y5P	1	0
17	AV	43	Y5P	6	0
47	BB	38	P5P	2	0
17	AV	51	Y5P	2	0
17	AV	36	P5P	2	0
47	BB	46	P5P	1	0
17	AY	11	Y5P	2	0
17	AY	71	Y5P	2	0
47	BB	62	Y5P	3	0
47	BB	44	Y5P	3	0
17	AV	11	Y5P	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AV	48	Y5P	2	0
17	AY	7	Y5P	2	0
17	AY	55	Y5P	14	0
47	BB	12	Y5P	1	0
17	AV	71	Y5P	1	0
17	AY	34	P5P	2	0
17	AY	36	P5P	2	0
17	AV	8	Y5P	1	0
17	AY	25	Y5P	6	0
17	AY	8	Y5P	5	0
17	AV	55	Y5P	7	0
17	AY	67	Y5P	3	0
17	AY	3	Y5P	3	0
17	AV	59	Y5P	2	0
17	AV	58	Y5P	4	0
17	AY	31	Y5P	3	0
47	BB	48	Y5P	1	0
47	BB	24	P5P	4	0
47	BB	13	Y5P	2	0
17	AV	63	Y5P	4	0
17	AV	62	Y5P	2	0
17	AV	41	Y5P	1	0
47	BB	26	Y5P	2	0
17	AY	24	Y5P	3	0
17	AV	37	Y5P	5	0
17	AY	68	Y5P	4	0
17	AY	56	Y5P	1	0
47	BB	47	P5P	1	0
17	AV	60	Y5P	2	0
17	AY	23	Y5P	1	0
18	AX	18	Y5P	2	0
17	AY	58	Y5P	11	0
17	AY	69	Y5P	2	0
17	AY	57	Y5P	3	0
17	AV	34	P5P	1	0
17	AV	57	Y5P	5	0
47	BB	65	Y5P	2	0
47	BB	28	P5P	3	0
17	AY	26	Y5P	3	0
47	BB	23	P5P	1	0
17	AY	42	Y5P	1	0
17	AV	3	Y5P	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	AV	64	Y5P	3	0
17	AY	54	Y5P	6	0
17	AV	32	Y5P	1	0
17	AV	42	Y5P	3	0
17	AV	70	Y5P	1	0
17	AV	28	Y5P	6	0
47	BB	66	P5P	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 358 ligands modelled in this entry, 357 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
91	GDP	Ag	500	-	29,30,30	1.35	2 (6%)	45,47,47	1.88	6 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	GDP	Ag	500	-	-	7/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
91	Ag	500	GDP	PA-O3A	3.73	1.63	1.59
91	Ag	500	GDP	C5-C4	3.65	1.48	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
91	Ag	500	GDP	C5-C4-N3	-6.42	118.18	128.39
91	Ag	500	GDP	C2-N3-C4	5.36	121.53	112.30
91	Ag	500	GDP	N9-C4-N3	4.71	135.38	125.95
91	Ag	500	GDP	C6-C5-N7	3.26	136.23	130.29
91	Ag	500	GDP	C4-C5-N7	-2.65	106.47	110.67

There are no chirality outliers.

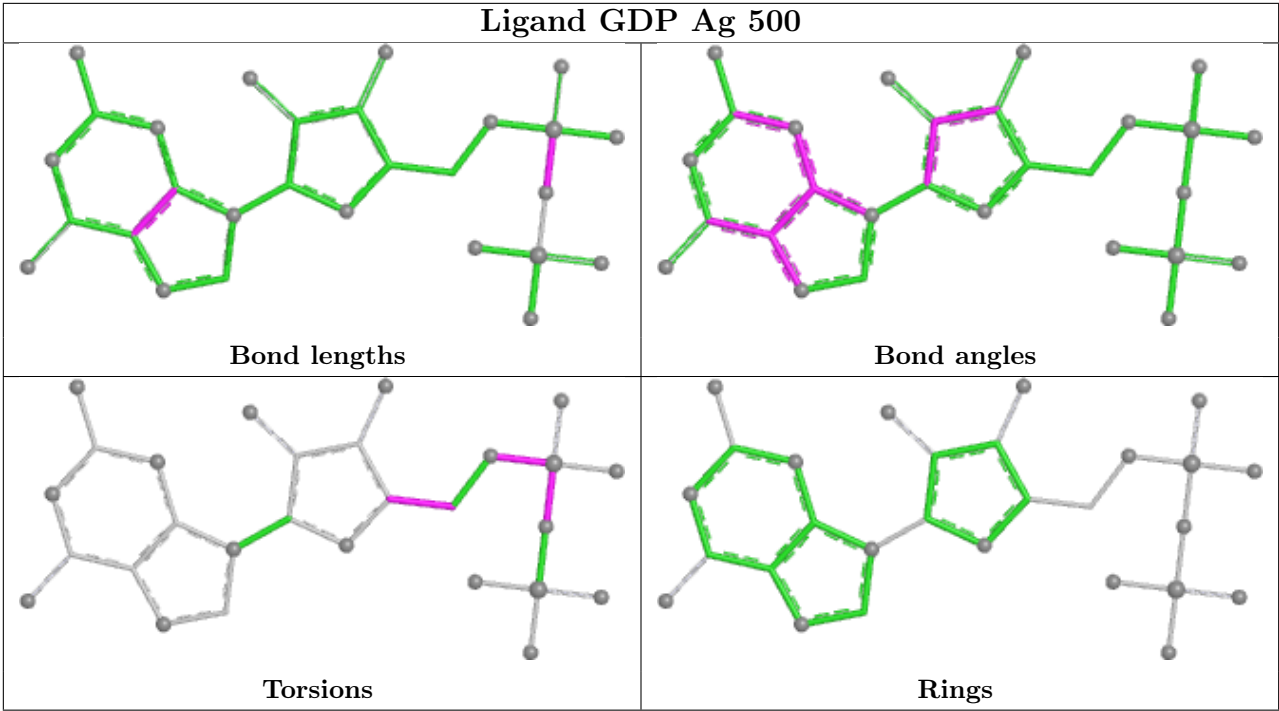
5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
91	Ag	500	GDP	C5'-O5'-PA-O3A
91	Ag	500	GDP	C5'-O5'-PA-O1A
91	Ag	500	GDP	C5'-O5'-PA-O2A
91	Ag	500	GDP	O4'-C4'-C5'-O5'
91	Ag	500	GDP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	Ao	26
88	Bz	4
23	Ae	4
17	AY	3
47	BB	2
17	AV	2
7	AI	1
4	AE	1

The worst 5 of 43 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	36:UNK	C	99:UNK	N	56.86
1	Bz	425:UNK	C	601:UNK	N	55.59
1	Ae	262:UNK	C	263:UNK	N	42.03
1	Ae	309:UNK	C	354:UNK	N	28.87

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Bz	106:UNK	C	300:UNK	N	28.46

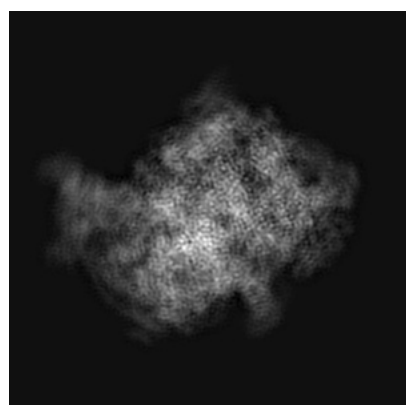
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2914. These allow visual inspection of the internal detail of the map and identification of artifacts.

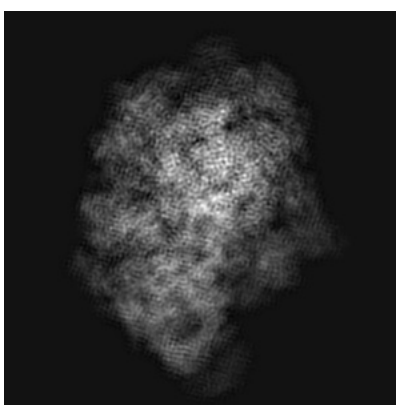
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

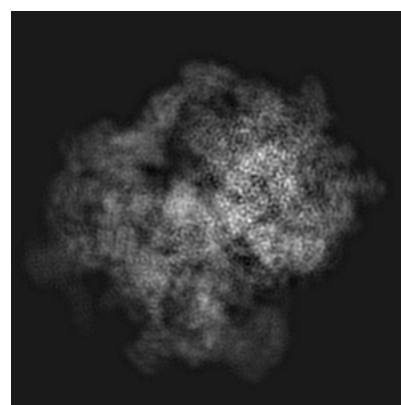
6.1.1 Primary map



X



Y

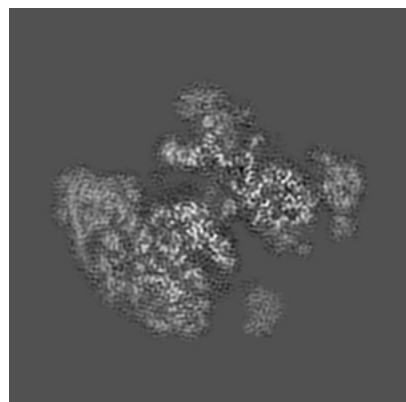


Z

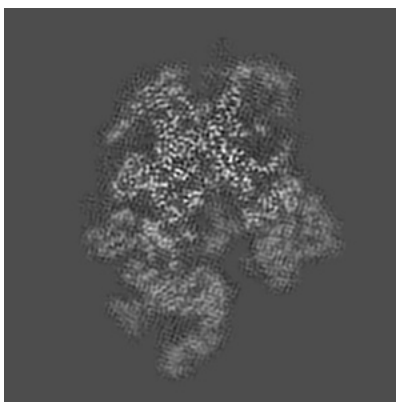
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

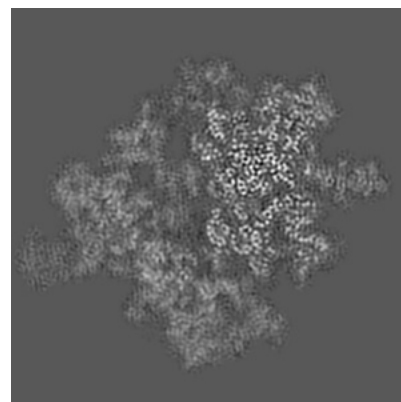
6.2.1 Primary map



X Index: 128



Y Index: 128

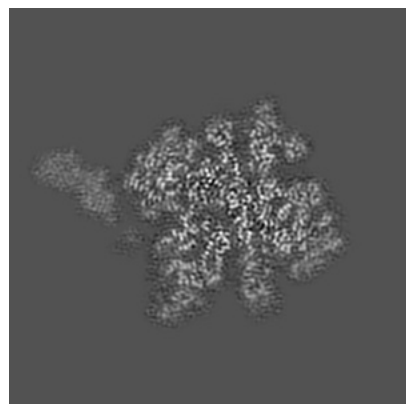


Z Index: 128

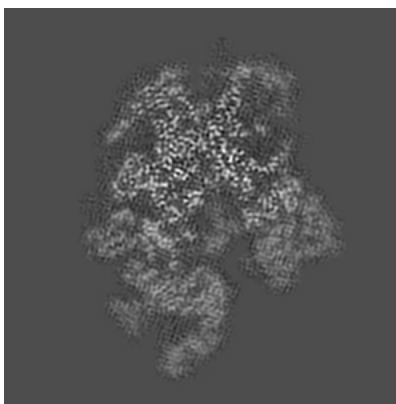
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

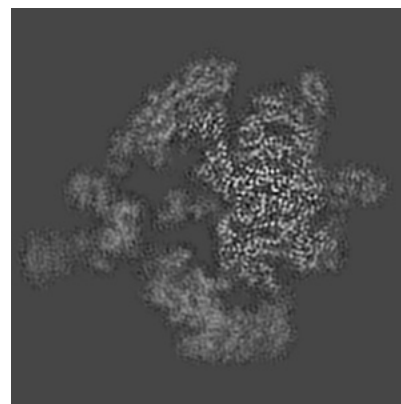
6.3.1 Primary map



X Index: 159



Y Index: 128

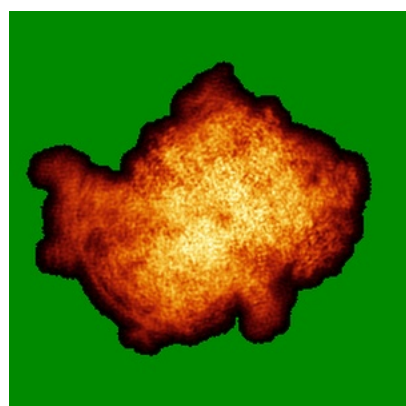


Z Index: 138

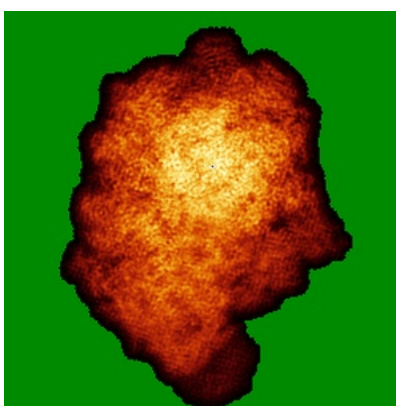
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

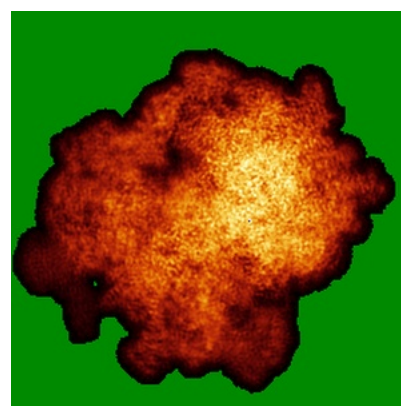
6.4.1 Primary map



X



Y

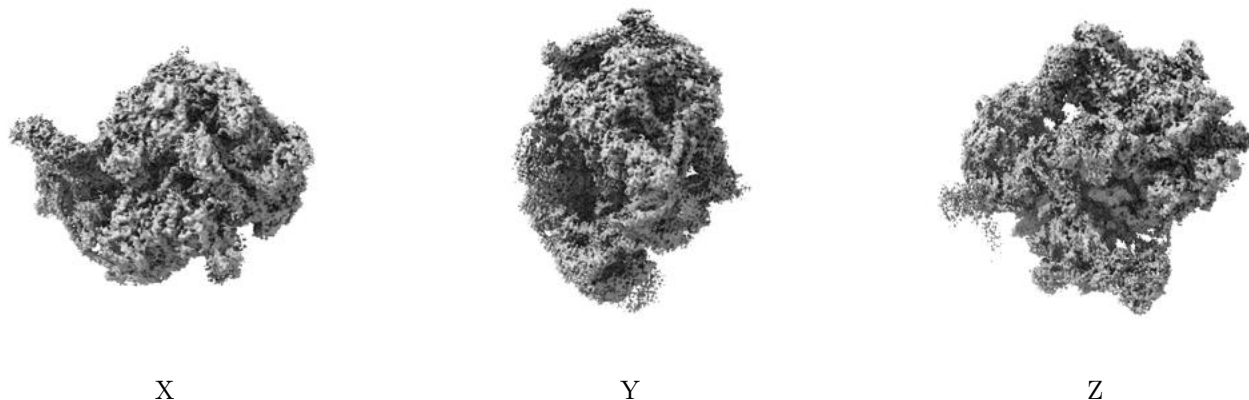


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

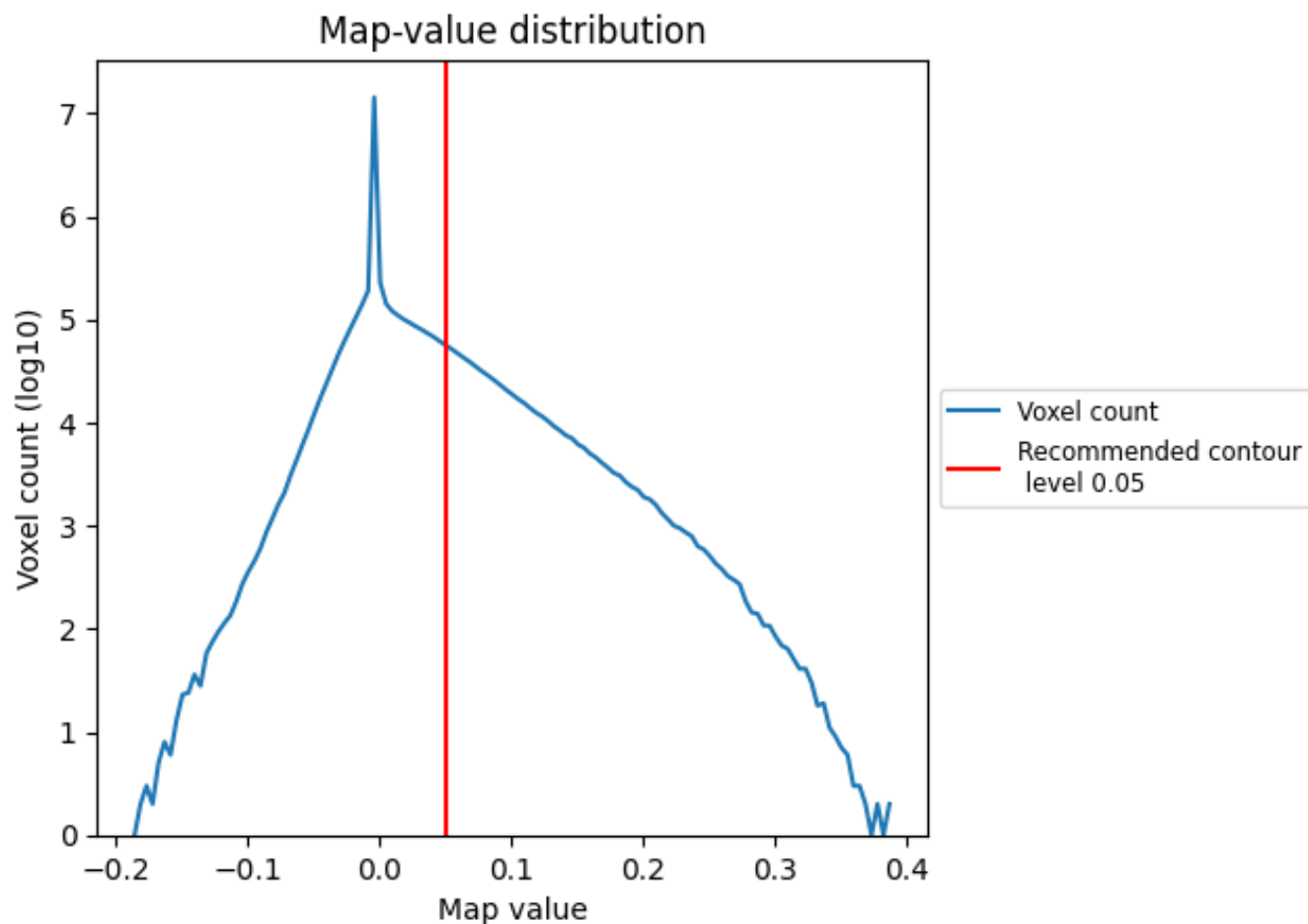
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

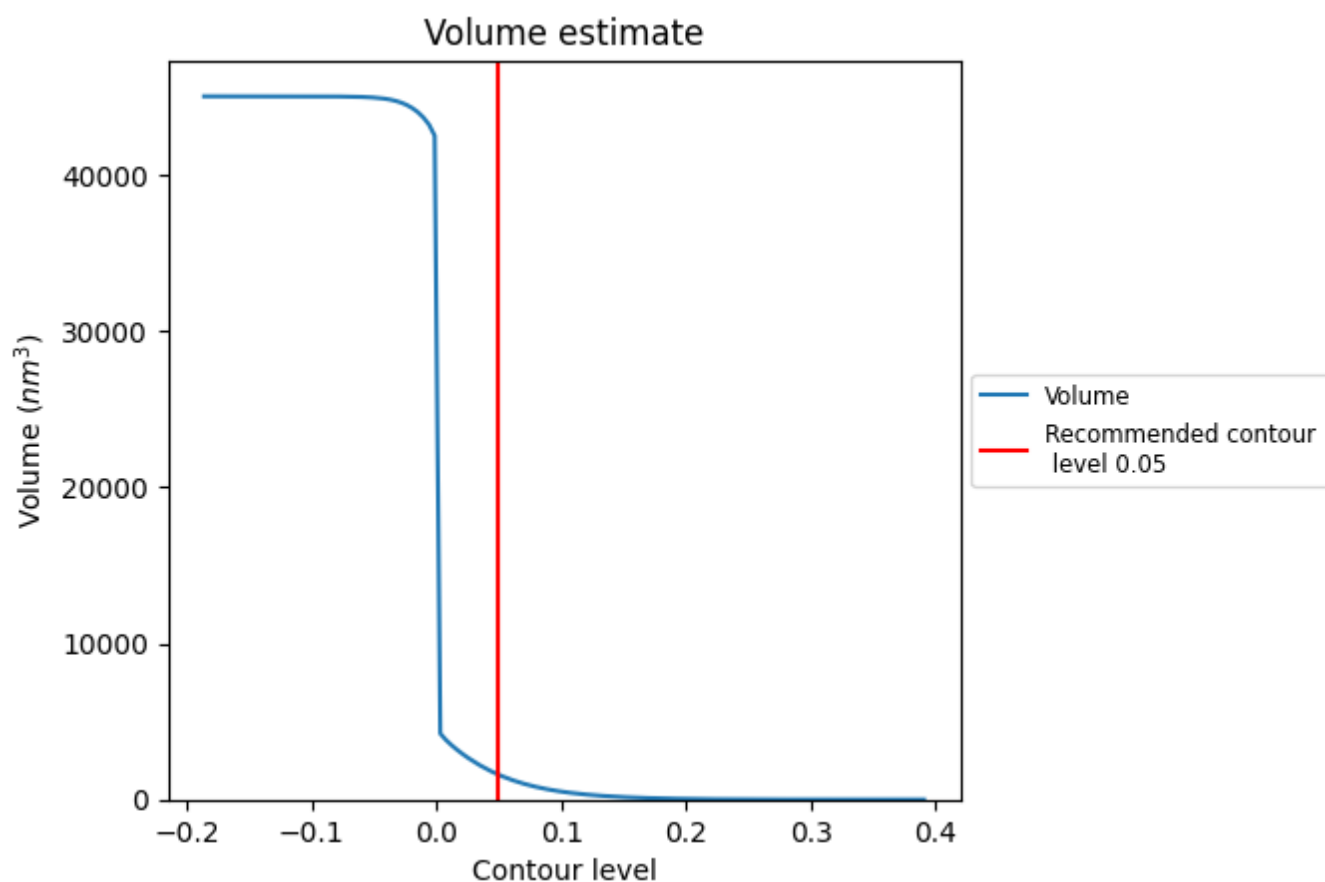
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

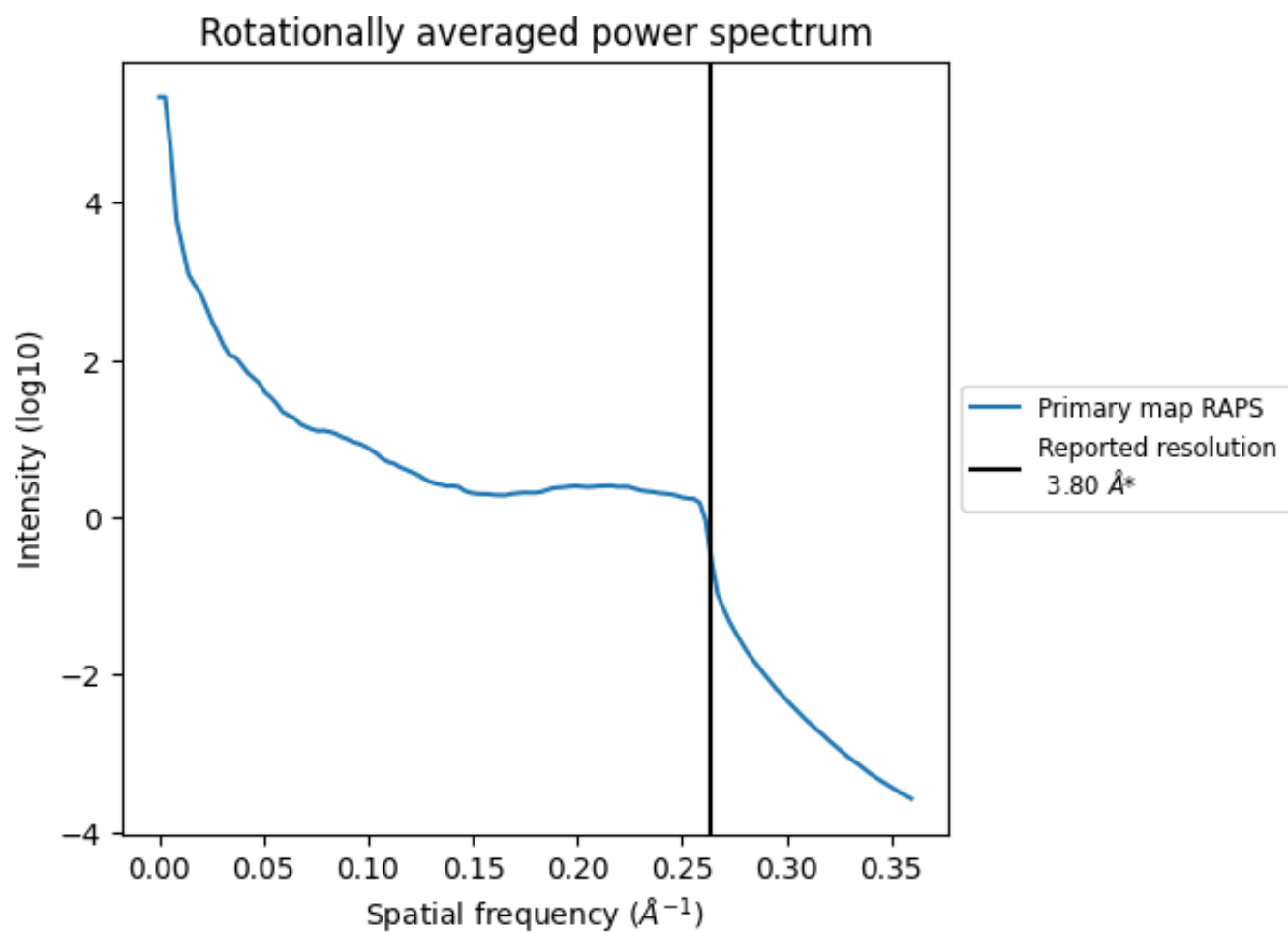
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1591 nm³; this corresponds to an approximate mass of 1437 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

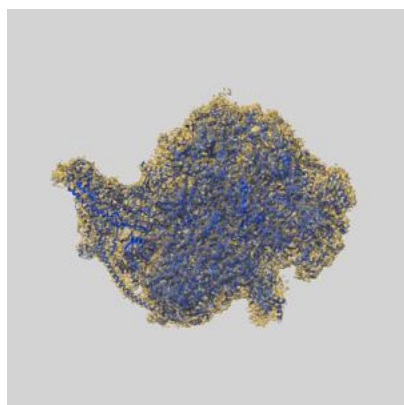
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

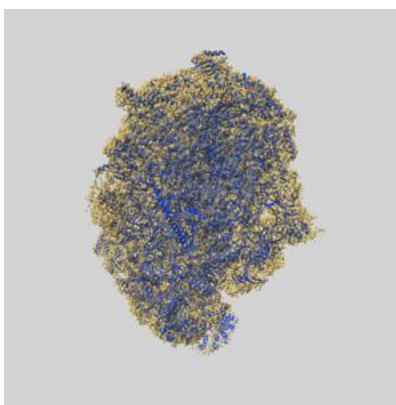
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2914 and PDB model 5AJ4. Per-residue inclusion information can be found in section [3](#) on page [23](#).

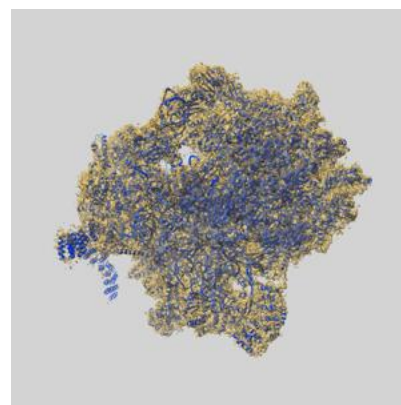
9.1 Map-model overlay [i](#)



X



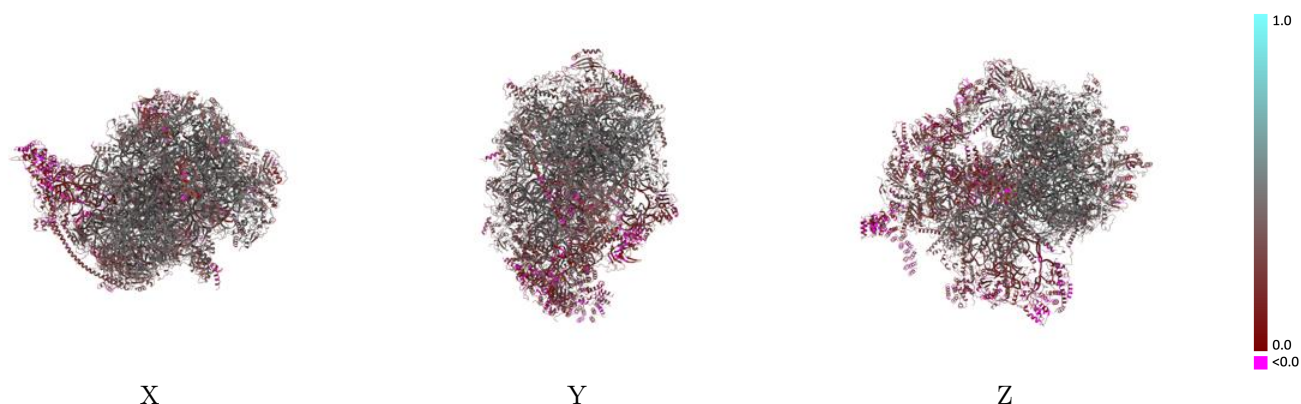
Y



Z

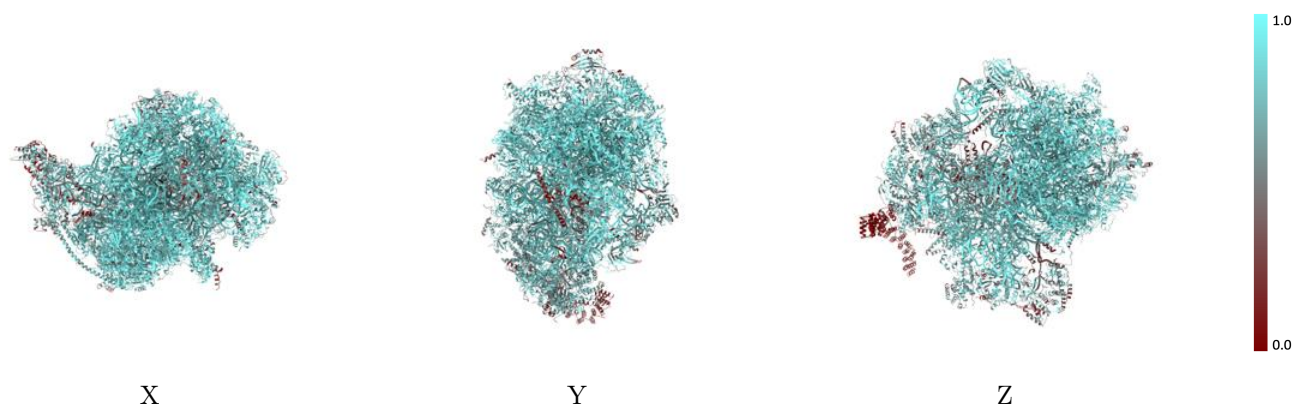
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



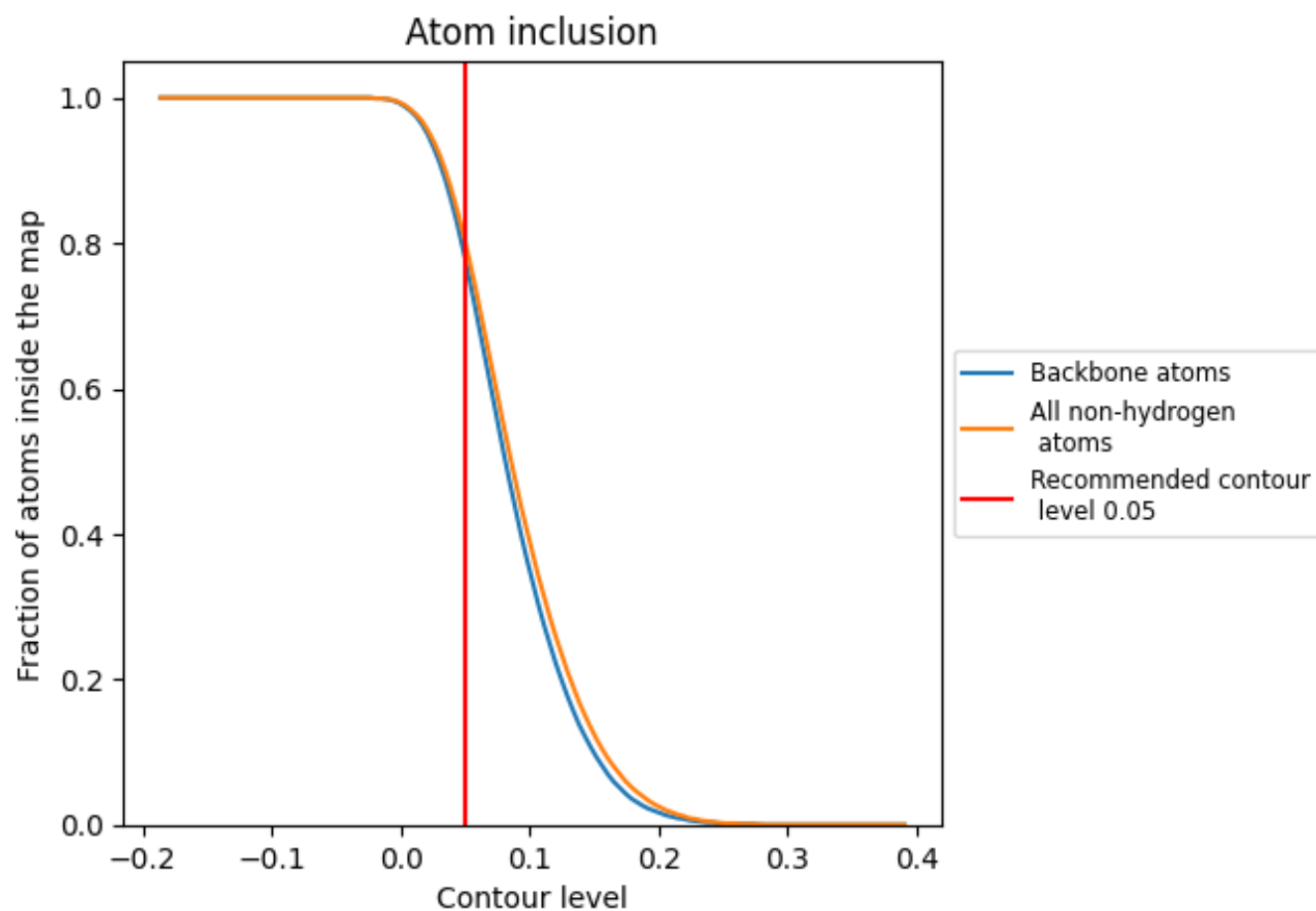
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.3580
AA	 0.9200	 0.3580
AB	 0.7920	 0.3500
AC	 0.7490	 0.3540
AE	 0.7070	 0.3400
AF	 0.7510	 0.3610
AG	 0.6430	 0.2620
AI	 0.7100	 0.2850
AJ	 0.7180	 0.2990
AK	 0.8160	 0.3670
AL	 0.7460	 0.3790
AN	 0.7890	 0.3120
AO	 0.7150	 0.3430
AP	 0.7240	 0.2080
AQ	 0.7940	 0.3420
AR	 0.7900	 0.3810
AU	 0.7950	 0.3760
AV	 0.6410	 0.2940
AX	 0.7490	 0.4000
AY	 0.4840	 0.2070
Aa	 0.6410	 0.1880
Ab	 0.6870	 0.2790
Ac	 0.7380	 0.3080
Ad	 0.7310	 0.2440
Ae	 0.5250	 0.1220
Af	 0.7290	 0.3360
Ag	 0.6800	 0.1920
Ah	 0.6970	 0.2250
Ai	 0.7280	 0.2650
Aj	 0.5360	 0.1580
Ak	 0.6560	 0.2400
Am	 0.6970	 0.3340
An	 0.7910	 0.4160
Ao	 0.2110	 0.1440
Ap	 0.7260	 0.2400



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Chain	Atom inclusion	Q-score
As	 0.0730	 -0.0030
Az	 0.7550	 0.2900
B0	 0.9010	 0.4720
B1	 0.8310	 0.4060
B2	 0.8590	 0.4290
B3	 0.8860	 0.4520
B4	 0.8340	 0.2750
B5	 0.8490	 0.4260
B6	 0.1900	 0.1820
B7	 0.9080	 0.4800
B8	 0.8970	 0.4840
B9	 0.9250	 0.4600
BA	 0.9540	 0.4350
BB	 0.8950	 0.2640
BD	 0.8810	 0.4570
BE	 0.8710	 0.4320
BF	 0.8920	 0.4530
BI	 0.7290	 0.3510
BJ	 0.6380	 0.2690
BK	 0.4930	 0.1750
BN	 0.8910	 0.4580
BO	 0.8690	 0.4550
BP	 0.8990	 0.4400
BQ	 0.8740	 0.4420
BR	 0.8780	 0.4480
BS	 0.8560	 0.3790
BT	 0.8230	 0.4230
BU	 0.8710	 0.4490
BV	 0.8490	 0.4390
BW	 0.8590	 0.4720
BX	 0.8510	 0.4360
BY	 0.6230	 0.3490
Ba	 0.8690	 0.4050
Bb	 0.8340	 0.3330
Bc	 0.8180	 0.3520
Bd	 0.7260	 0.2320
Be	 0.8260	 0.3880
Bf	 0.7790	 0.4070
Bg	 0.8900	 0.4590
Bh	 0.8320	 0.3890
Bi	 0.5600	 0.2960
Bj	 0.7040	 0.1810

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Chain	Atom inclusion	Q-score
Bk	 0.7420	 0.3210
Bl	 0.8990	 0.4350
Bm	 0.7690	 0.3240
Bn	 0.8900	 0.4730
Bo	 0.8610	 0.4180
Bp	 0.5970	 0.2170
Bq	 0.6390	 0.2510
Bt	 0.8870	 0.4650
Bu	 0.5420	 0.2520
Bv	 0.5470	 0.2740
Bw	 0.8630	 0.4070
Bx	 0.8200	 0.3960
Bz	 0.3940	 0.2010